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Love Canal Emergency Declaration Area Habitability Study: User's Guide to the Soil Assessment for Indicator Chemicals Integrated Data Base

CH2M Hill Southeast, Inc., Reston, VA

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Love Canal Emergency Declaration
Area Habitability Study

User's Guide to the Soil Assessment for Indicator Chemicals Integrated Data Base

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Directions to the use of the data collected during the Love Canal Emergency Declaration Area Soil Assessment for Indicator Chemicals are provided. The data is contained in a Statistical Analysis System (SAS) relational data base, comprised of ten separate SAS data sets. The data base is available from the U.S. Environmental Protection Agency Region II. The data base contains data from field, preparation laboratory, analytical laboratory, and data validation sources. Over 1.8 million cells of data are contained in the data base.

The user's guide gives an overview of the source system, file contents, and SAS data set structure, describes specific data sets, and discusses the combining of files. Appendices list the data elements contained the data base and provide formulas used in computations.

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User's Guide to the Soil Assessment for Indicator Chemicals Integrated Data Base

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1.0 Introduction

This document has been prepared to provide guidance to users of the integrated data base created during the Love Canal Emergency Declaration Area Habitability Study--Soil Assessment for Indicator Chemicals. Approximately 1.8 million cells of data are contained in the data base. The data base is a Statistical Analysis System (SAS) relational data base, comprising ten separate SAS data sets (i.e., files). The data base is available from the U.S. Environmental Protection Agency (EPA) Region II.

A description of the study, including sampling, analytical techniques, and the intended statistical use of the data, are contained in Volume III, Soil Assessment--Indicator Chemicals, of a five-volume series entitled Love Canal Emergency Declaration Area Habitability Study. These documents are available through NTIS, and the user is directed to Volume III for background on the study intent and implementation.

The user is cautioned regarding the use of this data. The study was designed for a very specific purpose, and the data was collected and verified in accordance with that purpose. Other uses of the data could lead to invalid and/or erroneous conclusions. Careful consideration of the study design, as documented in Volume III, Soil Assessment--Indicator Chemicals, is required in any determination regarding the appropriate vs. inappropriate uses of this data.

This user's guide is divided into eight sections and four appendices:

- The introduction, which gives an overview of the source systems, file contents, and SAS data set structure;
- Six sections, each describing specific data sets in the data base;
- An additional section on combining files, which describes logical relationships between the data sets in the data base;
- Appendix A which lists the data elements in the data base alphabetically;
- Appendix B which lists equivalent data elements contained in multiple data sets;
- Appendix C which provides the formulas used in the recomputation of final results; and
- Appendix D which describes box plots, a statistical data presentation technique used in the study.

1.1 Source Systems

Development of the data and information systems was built on the experience and software developed during a pilot soil study and the soil assessment for dioxin. In addition, a functional requirements analysis provided a software requirements summary and a data flow diagram (see Figure 1-1).

Ten separate software systems were used: eight were implemented on personal computers, and two were implemented on the EPA mainframe system. Ease of use and the editing capabilities to identify invalid data and prevent illogical functions were high priorities in the development of virtually all of the systems. A system flow chart depicting nine of these systems is presented in Figure 1-2. The tenth system (not shown) was a model data base implemented on the mainframe. The model data base was used to design and test the statistical analyses performed for the study. Each system is described in Table 1-1.

The construction of the Integrated Data Base incorporated many automated data verification checks. The flow of this process is shown in Figure 1-3. Table 1-2 lists the steps in the load and verification processes.

The resulting Data Base is organized into ten interrelated files.

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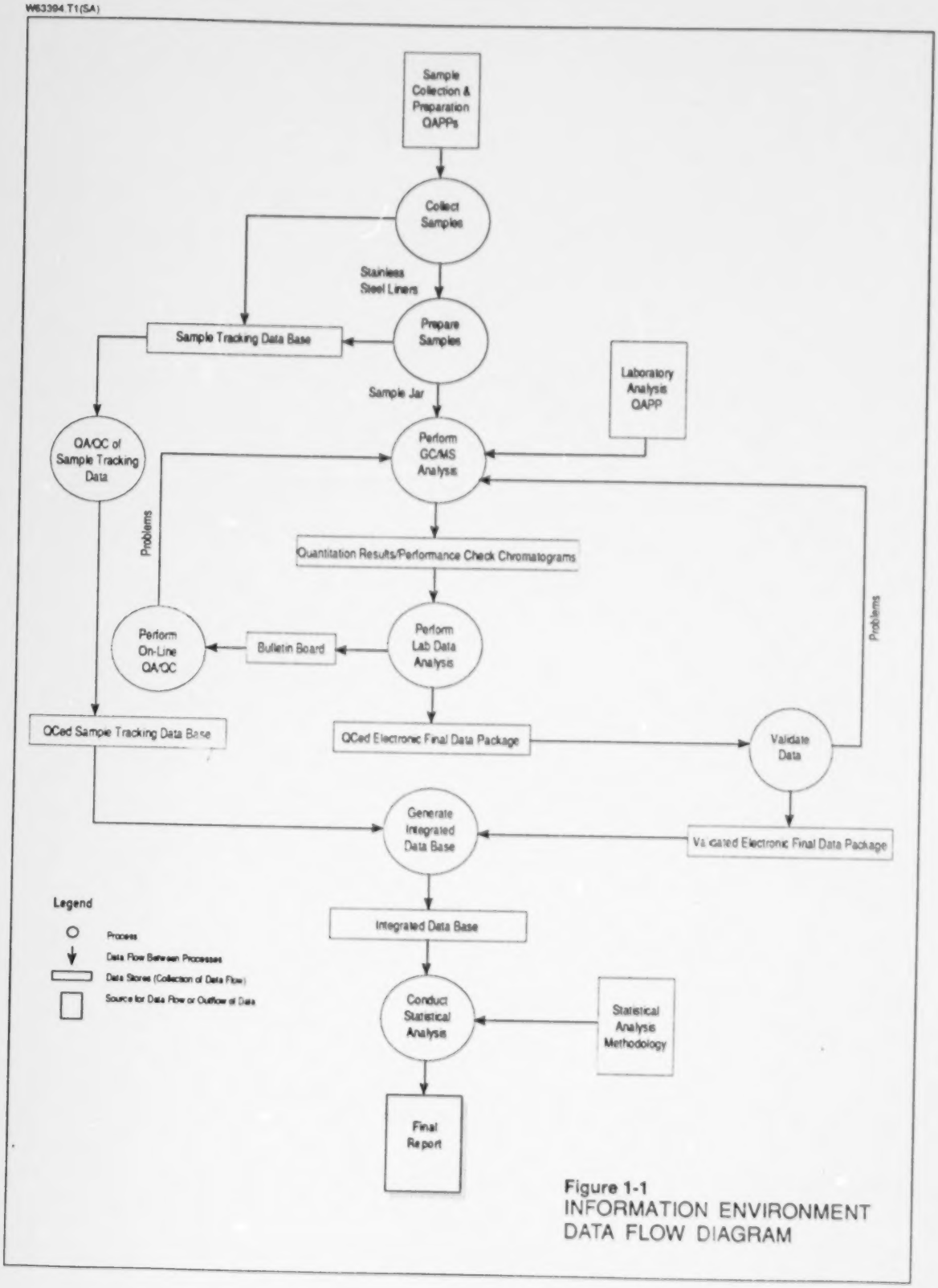

Figure 1-1
INFORMATION ENVIRONMENT
DATA FLOW DIAGRAM

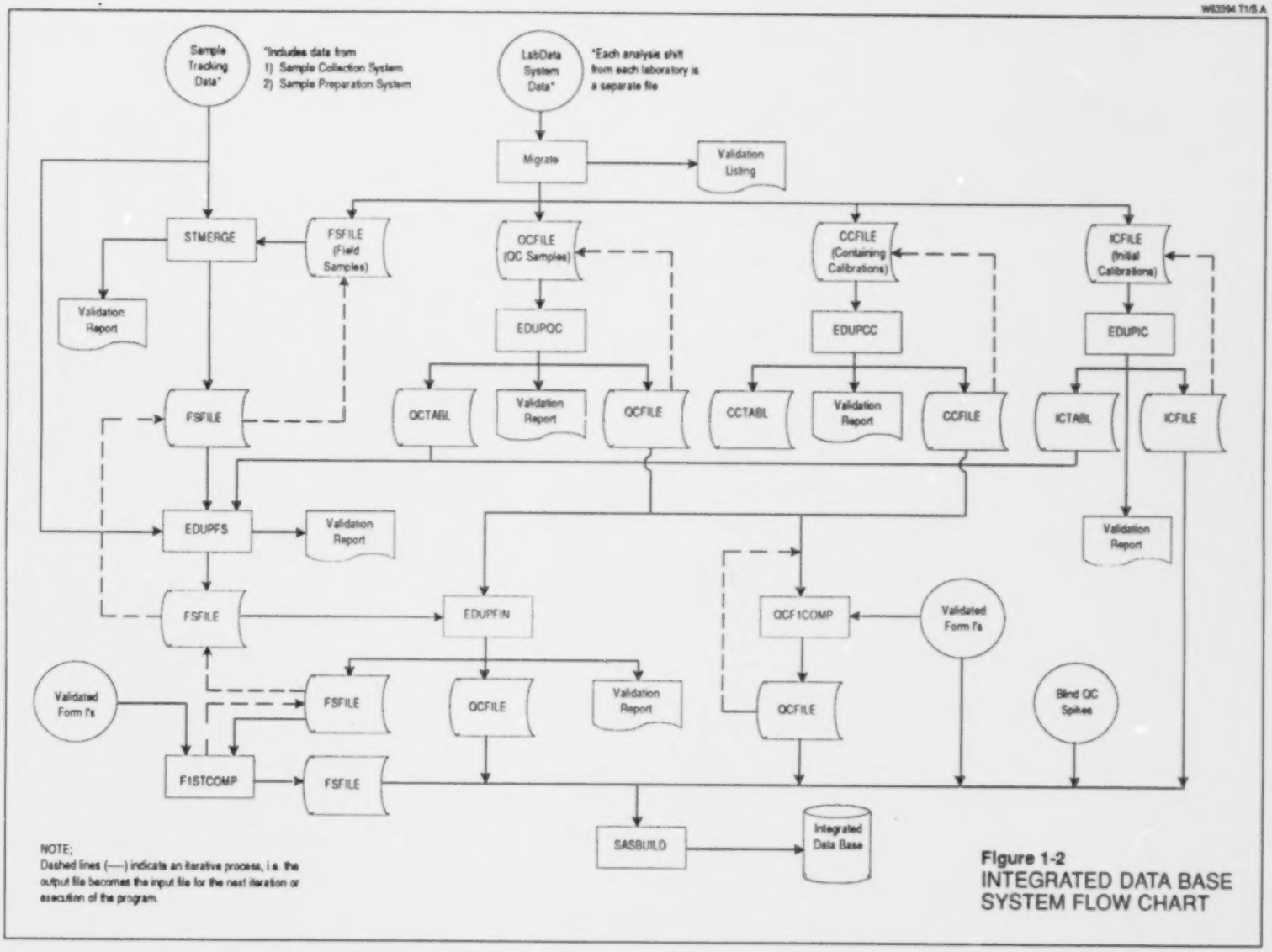

Figure 1-2
INTEGRATED DATA BASE SYSTEM FLOW CHART

Table 1-1

SOFTWARE SYSTEMS DEVELOPED AND USED IN THE SOIL ASSESSMENT FOR INDICATOR CHEMICALS

System Name	Description
Site Selection	- generates random selection sample locations on EDA grid and comparison area grid maps
Sample Collection	- generates forms and labels for field sampling, - collects completed forms (via double-data entry and comparison), - verifies data, and - produces reports on tracking/collection status
Sample Preparation	- generates and tracks sample preparation forms, - automatically generates the project sample identification number and indicates sample splits and target matrix spike/matrix spike duplicate (MS/MSD) samples, and - edits and verifies data entered on forms and produces labels and reports on preparation data status
Sample Analysis (LabData)	- generates sample analysis data reporting forms - performs chromatogram performance check analyses - provides automatic interface with project On-line QA/QC System - generates the electronic final data package, and - provides automatic interface with the project Data Validation System
Real-time QA/QC	- produces QC reports on samples being analyzed in the project laboratories on a real-time basis, and - produces daily control charts for selected QC data

Data Validation	- interfaces with the project LabData System and automatically displays analytical results to be reviewed, including shift files and calibration, - provides data entry for validation checklists, and - provides error and status reports
Form I Data Entry	- collects and verifies the Form I's (data reporting forms containing LCIC concentrations) validated by U.S. EPA Environmental Monitoring Systems Laboratory in Las Vegas (EMSL-LV), including the data validation and usability flags assigned, and - generates a file for uploading to the mainframe data base
Integrated Model Data Base	- creates a model SAS data base with selected fields filled with data, using distributions from the pilot study
Integrated Data Base	- integrates the data generated from the LabData, Sample Collection, Sample Preparation, Data Validation, and Form I Data Entry systems into a mainframe SAS data base, - recalculates all data reported on the LabData forms, - checks for data consistency between the systems where the same data were available from more than one source, and - reports discrepancies and omissions
Project Bulletin Board	- provides both file uploading and downloading capabilities with full security features for interfacing of project systems, and - provides a message center for automated transfer of information between geographically dispersed project staff

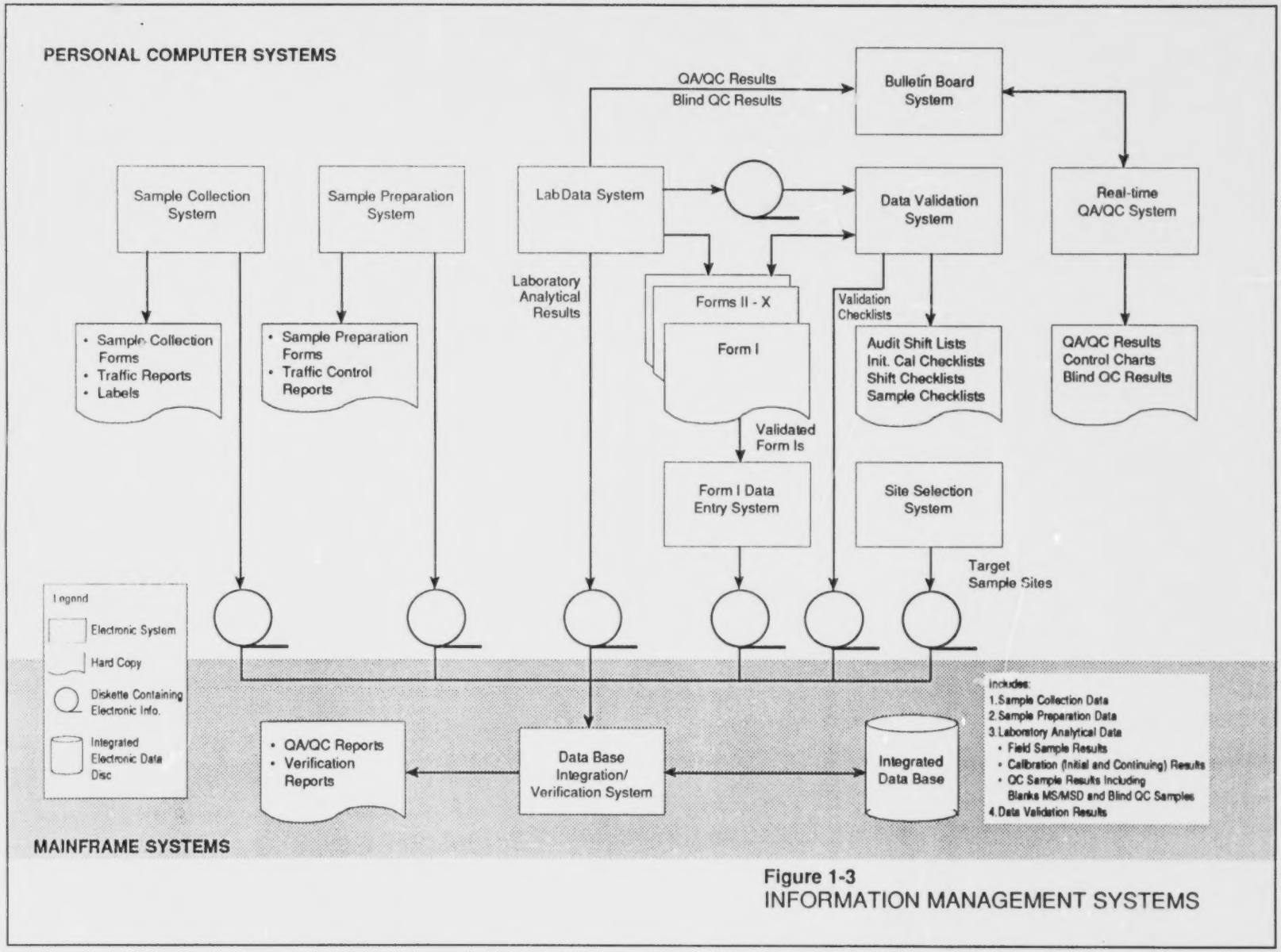

Figure 1-3
INFORMATION MANAGEMENT SYSTEMS

Table 1-2

STEPS IN THE LOAD AND VERIFICATION PROCESS

	Program Name	Description
1.	Validate LabData (manual process)	The lists prepared by EMSL-LV during the data validation process were used during visits to each laboratory to verify that the laboratory's LabData System data conformed to the list. (This list, organized by analysis shift, details all validated analyses, including calibrations and field QC analysis.) After completion of the verification, final data packages for all valid analyses shifts were then generated.
2.	Upload Final Data Packages (manual process)	The final data packages, contained on diskettes, were uploaded to the EPA mainframe computer. All files were successfully uploaded.
3.	MIGRATE	The MIGRATE program, which separated the LabData data into separate files to be loaded into the integrated data base, was then executed.
4.	STMERGE	The program that merged the sample tracking data with the field sample data was executed. The validation report from this program listed records in sample tracking that did not match to a field sample from the LabData System and vice-versa. All discrepancies were resolved.
5.	EDUPQC	This program processed the QC samples and recomputed results fields, using the original quantitation report data, generated by LabData. Only results fields requiring no data from other quantitation reports (e.g., calibration data) were recalculated. All discrepancies were resolved in fields used to join other table entries.

6.	EDUPIC	This program processed the IC samples and recomputed results fields using the original quantitation report data generated by LabData. All discrepancies were resolved.
7.	EDUPCC	This program processed the CC samples and recomputed results fields using the original quantitation report data generated by LabData. Only results fields requiring no data from other quantitation reports (e.g., IC data) were recalculated. All discrepancies were resolved in fields used to join other table entries.
8.	EDUPFS	This program processed the field samples and recomputed selected results fields using the original quantitation report data generated by LabData. Only results fields requiring no data from other quantitation reports (e.g., calibration data) were recalculated. Sample IDs were verified against the sample tracking data. Edits were performed to verify that the calibration entry for the field sample was in the data base and that QC samples pointed to by the field sample were also in the data base. All discrepancies were resolved in fields used to join other table entries.
9.	EDUPFIN	This program processed the field samples, verifying all fields that require data from multiple sources; it recomputed concentrations, recoveries, etc., and all discrepancies were resolved.
10.	FISTCOMP QCSTCOMP	These programs performed a three-level match between the Form I data validated by EMSL-LV and the data entered and the Form I data contained on LabData. The initial match was on the Lab Login identification for the Form I. This was the unique key used by the LabData System to track the sample analysis. Any mismatches were reported. Then, for those samples whose identifications matched, two additional levels were checked. The sample identification (the project identification), analysis date, and

	analysis time were matched and mismatches reported. Then all LCIC concentrations, percent moisture, and dilution factors were compared. Discrepancies between Lab Login IDs were resolved, validated Form I's were linked to a valid LabData entry (which contains all the raw data for the analysis), and all LabData entries were linked to a validated Form I.
11. SASBUILD	This program loaded the validated data files into the integrated data base.

1.2 Contents of Files

The Integrated Data Base is composed of six master files and four ancillary files, as follows:

- Field Sample Master File and Ancillary File,
- Initial Calibration Master File and Ancillary File,
- Continuing Calibration Master File and Ancillary File,
- Quality Control Sample Master File and Ancillary File,
- Form1 Master File, and
- Blind Quality Control Spike Master File.

Prior to processing data files it is often useful to know how many records they contain. Following are the record counts for the master files:

Master File	Records
FSFILE	58
ICFILE	239
CCFILE	1443
QCFILE	534
F1FILE	1564
BQFILE	293

Each of the master files is discussed below. Each ancillary file corresponds to a master file and contains the original values for GC/MS data corrected by the analyst via the LabData Corrections subsystem. A record exists in an ancillary file only when one or more of the Area/Scan Retention Time correction flags in the master file are "on," indicating that a correction has been made. For example, a value of "Y" in the FSCANAL data element (correction flag for analyst) indicates that the Field Sample Master File contains corrected data in the FSANLST data element. It also indicates the existence of a record in the Field Sample Ancillary File, containing the original (uncorrected) data.

An ancillary file has the same key field as its master file and, except for the IC and CC ancillary files, the same SAS data field names. Note that the master files contain the corrected data while the ancillary files contain the original data.

The logical hierarchy of the data is as follows:

```
INITIAL CALIBRATION
     CONTINUING CALIBRATION
          FIELD SAMPLES
          QC SAMPLES
     CONTINUING CALIBRATION
          FIELD SAMPLES
          QC SAMPLES
     .
     .
     .
INITIAL CALIBRATION
     CONTINUING CALIBRATION
          FIELD SAMPLES
          QC SAMPLES
.
.
.
```

As can be seen, one Initial Calibration can have one or more Continuing Calibrations associated with it; one Continuing Calibration can have one or more Field and/or QC Samples associated with it.

Field Sample Master File

A record in the Field Sample Master File contains all sample collection, sample preparation, and GC/MS analysis data for all field samples (HS), field splits (SPLIT), holding time samples (HT), field handling blanks (FHB), preparation handling blanks (PHB), and PHB splits. The GC/MS analysis data includes all quantitation report data and computed data for the sample analysis. Field samples are the soil samples actually taken from the ramdomly selected locations in the various sampling areas. Field splits are created by splitting a field sample in a manner controlled to maintain representativeness. One half is treated just as any other field sample, and the other receives a new project sample ID (i.e., "HS" number). The results from the two halves can then be used to assess inter- and intra-laboratory variability.

Field handling blanks were "double blind" Quality Control (QC) samples that were sent to the analytic laboratories just as field samples were. The field handling blanks were samples of uncomtaminated soil with an appearance similar to the field sample soil. (The soil used for the blanks was taken from a larger volume of soil that had been analyzed to verify that no measurable concentrations of LCICs were present.) The field handling blanks were used to measure whether cross-contamination had occurred during the shipment, sampling, preparation, and analytical processes. The field handling blanks were considered "double blind" QC samples, because neither their identity nor the

concentration of LCICs present was revealed to the analytical laboratory.

Preparation handling blanks (PHB) and PHB splits were QC samples that were sent to the analytic laboratories along with the field samples. They were not analyzed unless contamination was measured in the field handling blank.

Holding time samples were aliquots of soil samples used to study the effects of extending the sample holding time on LCIC concentrations in the samples.

Pointers, or keys, are present to join each sample's initial calibration record, continuing calibration record, method blank record, matrix spike (MS) and matrix spike duplicate (MSD) records (if any), and Form I record.

Initial Calibration Master File

In the Initial Calibration Master File, a record contains all quantitation report data and computed data for each five-point initial calibration and/or EPA performance check analysis run on the GC/MS. The performance check analysis could be run either in the same analytic run (i.e., "shift") as the five-point or in a later shift. Therefore some records contain the five-point data and the performance check data; some records, only the five-point data; and some records, only the performance check data. Logically, this data represents the top of the data structure. All continuing calibrations are associated with a five-point initial calibration; thus one or more continuing calibration records will point to a single initial calibration record.

Continuing Calibration Master File

In the Continuing Calibration Master File, a record contains all quantitation report and computed data for each performance check 1/continuing calibration analysis and performance check 2 analysis run for an analytic shift on the GC/MS. This data represents the second logical level in the data structure. Each continuing calibration record will have one or more field sample and/or QC sample records pointing to it.

Quality Control (QC) Sample Master File

In the QC Sample Master File, a record contains all quantitation report and computed data for QC samples. Each analytic run, or "shift," containing field samples was required to have certain QC samples run as well. Depending upon various factors, one or more types of QC samples were run in each shift. The QC samples include the following types:

1) EMSL Blind QC samples - These were "single blind" samples spiked with known concentrations of LCICs. The samples are considered "single blind" to the laboratory

because although the laboratory knows which samples are Blind QC samples, the laboratory does not know the spiked concentration of LCICS. A Blind QC sample was extracted with each extraction batch of samples and analyzed. If a given level of recovery was not achieved in the Blind QC sample, then the laboratory was directed to re-extract and re-analyze all the field samples in the extraction batch.

2) Matrix Spike and Matrix Spike Duplicate - Approximately every twentieth field sample was split into three parts. One-third was treated as a normal field sample, called the "native" sample in a native/MS/MSD set of analyses. Each of the remaining thirds was then spiked with a fixed amount of LCICs. One was called a Matrix Spike (MS) and the other was called a Matrix Spike Duplicate (MSD).

3) Method Blank - This was a blank sample, prepared by the analytic laboratory from soil that had been analyzed to verify that no measurable concentrations of LCICs were present. The sample was used to measure any cross-contamination during the analytical process. The sample was extracted in a batch of field samples, subjected to the same laboratory handling and storage procedures, and analyzed with the field samples. If significant levels of LCICs were found, the laboratory re-extracted and re-analyzed the field samples in that extraction batch.

4) Reagent Blank - This was a blank sample extract, made from the solvents used during the sample extraction process. The extract was analyzed to measure any LCIC contamination introduced into the field samples during the sample extraction process.

A pointer, or key, is present to link to each sample's continuing calibration record.

Form I Master File

In the Form I Master File, a record contains Form I data validated by EMSL-LV, along with flags indicating validation and usability. The Form I document reports LCIC concentrations. The Form I's were generated by the LabData system at the laboratory. Both the electronic and the hardcopy results were transmitted by the laboratory to EMSL-LV for cross-checking and for data validation. The results of the cross-check and data validation were incorporated in the Form I Master File.

The EMSL-LV data validation was an extensive review of the Form I results, verifying that the concentrations on the Form I were correctly reported. It included a review of both the data and

supporting documentation produced by the analytic laboratories. A series of flags was developed to characterize the data, and from these flags, a summary usability flag was assigned. A complete description of this process is contained in Appendix H of Volume III. Because of this extensive review, the Form I data contained in the Form I Master File are considered the "official" results.

(The terms "Form I" and "Form1" are used interchangeably in this document.)

Blind QC Spike Master File

In the Blind QC Spike Master File, each record contains analyte spiking levels for the blind QC sample sent by EMSL-LV to the analytical laboratory.

1.3 The Structure of a SAS Data Set

The Integrated Data Base is stored in a SAS data library. The SAS System is a software system for data analysis. Each of the "files" in the Integrated Data Base is a SAS data set within the data library.

A SAS data set is a collection of data values arranged in a rectangular form as shown in Figure 1-4. Each cell in the rectangular table is a data value. The data values associated with a single entity - a sample, a record - make up an observation. In Figure 1-4, each row represents one observation. The first observation represents all the data values associated with the first sample whose data was recorded. The last observation represents all the data values for the last sample. In this document, the word "record" will often be used in place of the SAS term "observation."

XXKEY	XXY1	XXY2	XXY3	XXY4	XXY5	XXY6
A0001	1	2	3	4	5	6
A0003	101	202	303	404	505	606
A0008	111	222	333	444	555	666
A0009	11	22	33	44	55	66

Figure 1-4: A SAS Data Set

The set of data values that describe a given characteristic make up a "variable." Each observation in a SAS data set contains one data value for each variable. In Figure 1-4, each column of data values is a variable. For example, the first column makes up the variable XXKEY and contains all the keys of the samples in the data set, the second column makes up the variable XXY1 and contains the sample's Y1's, and so on. The term "variable" has

been replaced with "data element" in other sections of this document.

There are two types of SAS variables: numeric and character. SAS variables have a length attribute and a label attribute. The length attribute of a variable is the number of bytes used to store each of its values in a SAS data set. The label attribute is a descriptive label that can be printed by certain SAS procedures instead of the variable name. Labels have been stored with the variables in the Integrated Data Base.

Many of the SAS data elements in the Integrated Data Base are components of "arrays." The elements shown in Figure 1-4 called XXY1 through XXY6 could be defined to SAS as a two-dimensional array with two rows and three columns. This would be accomplished by coding a SAS statement as follows:

```
ARRAY XXY(2,3) XXY1-XXY6;
```

One might visualize the first record's XXY array as follows:

	column 1	column 2	column 3
row 1	1	2	3
row 2	4	5	6

The value of XXY(1,2) is 2, while the value of XXY(2,1) is 4. For further discussion of SAS arrays please refer to the SAS Users Guide: Basics, Version 5 Edition, Cary, NC: SAS Institute Inc., 1985.

1.4 Data Element Coding Standards

The Integrated Data Base includes 1.8 million "cells" of data. Many of the data elements are similar in the kind of data they represent. The following data element coding standards were adopted to make analysis of the data as easy as possible for the user.

Flags

Flags that represent binary choices, such as yes/no, contain "*" for yes-type responses and " " for no-type responses, except where otherwise documented.

Validation Audit Failures

Data elements marked with an "*" in the "source" column of the data elements descriptions have been recalculated during the data base building process. The results were checked against the output of LabData. Any record with a non-match between at least one LabData captured value and its recalculated value was flagged as a validation audit failure. The data element xxSTATUS was set

to "E," where xx indicates the file (e.g., FSSTATUS was in the Field Sample Master File).

Unique Key

The unique key in all files is the Analysis Lab Sample ID. This data element is of the form xxANALID, where xx varies by file.

LCICs

When a data element occurs for each LCIC, the description says "by 8 LCICs." The occurrences of the LCICs from 1 to 8 are as follows:

LCIC	Common Abbreviation
1 = 1,2-Dichlorobenzene	DCB
2 = 1,2,4-Trichlorobenzene	TCB
3 = 1,2,3,4-Tetrachlorobenzene	TeCB
4 = 2-Chloronaphthalene	CNP
5 = Alpha-BHC	A-BHC
6 = Delta-BHC	D-BHC
7 = Beta-BHC	B-BHC
8 = Gamma-BHC	G-BHC

Surrogates

When a data element occurs for each surrogate, the description says "by 3 surrogates." The occurrences from 1 to 3 are as follows:

Surrogate	Common Abbreviation
1 = 1,4-Dibromobenzene	DBB
2 = 2,4,6-Tribromobiphenyl	TBBP
3 = 1,2,4,5-Tetrabromobenzene	QBB

Internal Standards

When a data element occurs for each internal standard, the description says "by 5 Int Stds." The occurrences from 1 to 5 are as follows:

Internal Standard	Common Abbreviation
1 = D4-1,4-Dichlorobenzene	IS1
2 = D8-Naphthalene	IS2
3 = D10-Acenaphthalene	IS3
4 = D10-Phenanthrene	IS4
5 = D10-Pyrene	IS5

SAS Dates

The dates in the Data Base are stored as SAS dates. Each date is represented by the number of days between January 1, 1960 and that date. The SAS language allows for flexibility in printing dates in many recognizable forms.

1.5 Detailed Description of Individual File Sections

The remaining sections of this document provide detailed descriptions of the files that compose the Integrated Data Base. Each of these sections has three subsections, which contain the following information:

n.1 Logical Record Description - a narrative description of the logical records in the file, including counts, sort sequence, and data element groupings

n.2 Logical Subsets of the File - a discussion of subsets of the logical records in the file, including illustrations of data elements to be used for typical screening criteria

n.3 Data Element Dictionaries - detailed information about every data element in the file, presented in subject-related groupings. This information is given in tabular form, with column heading as follows:

Data Element ID - ID of the form AA.Bnn, where:
AA is an abbreviation of the file,
FS = Field Sample Master File
FA = Field Sample Ancillary File
IC = Initial Calibration Master File
IA = Initial Calibration Ancillary File
CC = Continuing Calibration Master File
CA = Continuing Calibration Ancillary File
QC = Quality Control Master File
QA = Quality Control Ancillary File
F1 = Form 1 Master File
BQ = Blind Quality Control Master File
B is an alphabetical character assigned to a data element group, and
nn is sequentially assigned within a data element group

Name - SAS data element name

Type - type of data element:
CHAR for character, or
NUM for numeric

Length - number of bytes used to store the data element

Dimensions (for arrays) - shows the number of dimensions for the data element array and the number of elements in each dimension [e.g., (8,3) is a two-dimensional array with 8 rows and 3 columns]

Description - text description of the data element, including "by" phrase(s) to describe any array dimensions (e.g., by eight LCICs)

Source System - identifies the system that provided the data element values, either captured/reported or computed (marked with a "*" prefix). Appendix C contains the formulas that were used in the computations.

2.0 Field Sample Master File and Ancillary File

A record in the Field Sample Master File contains all sample collection, sample preparation, and GC/MS analysis data for all field samples (HS), field splits (SPLIT), holding time samples (HT), field handling blanks (FHB), preparation handling blanks (PHB), and PHB splits.

Field samples were the soil samples actually taken from the ramdomly selected locations in the various sampling areas.

Field splits were created at the preparation laboratory by splitting a field sample in half. One half is treated just as any other field sample, and the other receives a new project sample ID (i.e., "HS" number). The results from the two halves could then be linked for inter- or intra-laboratory comparisons.

Holding time samples were soil samples used to study the effects of extending the sample holding time on LCIC concentration.

Field handling blanks were "blind" quality control (QC) samples of uncontaminated soil. These samples were used to measure cross-contamination of field samples throughout the shipping, sampling, preparation, and analytical procedures.

Preparation handling blanks and PHB splits were QC samples of uncontaminated soil that were sent to the analytic laboratories along with the field samples. They were not analyzed unless cross-contamination was measured in the field handling blanks.

Pointers, or keys, are present to join each sample's initial calibration record, continuing calibration record, method blank record, matrix spike (MS), and matrix spike duplicate (MSD) records (if any), and Form I record.

2.1 Logical Record Description

A logical record in this file contains data for one sample. The data elements are organized in groups, as follows:

- KEYS AND STATUS - the primary, unique identifier of each record in the file, along with any other (perhaps non-unique) keys, and the status flag.

- INTER-FILE LINKS/SECONDARY KEYS - Pointers, or keys, providing linkage to the following records in other files related to a sample: initial calibration, continuing calibration, method/holding blank, MS/MSD (if any), Form I, and blind QC.

- INTRA-FILE LINKS/SECONDARY KEYS - Pointers, or keys, providing linkage to records in this file related to a sample.

- CHRONOLOGY - dates and times of significant events during the processing of the sample.

- DATA TRANSFER TRACKING - system dates used for maintenance of the data base.

- FIELD SAMPLING DATA - data generated during the collection of the sample in the field.

- PREPARATION LAB DATA - data generated during the preparation of the sample. The preparation process consisted of removing the soil from the sampling tube, homogenizing the soil, placing the soil in a container for shipment, and shipping to an analytical laboratory.

- ANALYSIS LAB SAMPLE LOGIN DATA - data entered by the analytic laboratory when the sample was logged into their facility.

- ANALYSIS LAB SAMPLE EXTRACTION DATA - data generated by the analytic laboratory during the sample extraction process. This process removes the organic compounds from the solid soil material, resulting in a liquid suitable for analysis on the GC/MS.

- ANALYSIS LAB INJECTION DATA - data entered by the lab relating to injection of the sample in the GC/MS.

- ANALYSIS LAB INTERPRETATION DATA - data identifying the shift results file that the sample belonged to, the quantitation method used for each analyte, and the ion used for quantitation for each analyte. This data also contains the results of the GC/MS analysis when the peak height method of quantitation was used.

- CORRECTION FLAGS - flags used to indicate whether or not a particular element has been corrected/updated. If a flag is set "on" ("Y"), then the updated data is contained in this file, and the original data value is stored in the ancillary file record.

- ANALYSIS RAW DATA - (after corrections, if any) raw data generated by the GC/MS. This is essentially the same data contained on the quantitation report created by the GC/MS.

- LABDATA COMPUTATIONS FOR FIELD SAMPLES - results calculated by the LabData system using the raw data generated by the GC/MS and additional data entered by the laboratory. It includes the concentration results after the identification criteria (ID) have been applied, pre-criteria concentrations, ID criteria results, and flags indicating whether or not the criteria were met.

- LABDATA COMPUTATIONS FOR SURROGATE STANDARDS - results computed by LabData for the surrogate recoveries for the sample analysis. Included are the percent recoveries, flags indicating whether or not the recovery met the criteria, and the criteria.

- LABDATA COMPUTATIONS FOR INTERNAL STANDARDS - results computed by LabData for the internal standards for the sample analysis. Included are retention time and area criteria check results.

- DATA VALIDATION FLAGS AND COMMENTS - results of the data validation for the sample performed by EMSL-LV. It includes data validation checklist responses, comments, validation flags, and EMSL-LV usability flags.

- INTEGRATED DATA BASE AUDIT SYSTEM FLAGS - results of the automated audits and validations performed during the data base building process.

The ancillary file consists of three groups: KEYS, CHRONOLOGY, and DATA REPLACED BY CORRECTIONS. The last group corresponds to the ANALYSIS RAW DATA group in terms of data elements, but contains original data that has been replaced in the master file by corrected data.

2.2 Logical Subsets of the File

The primary grouping of logical subsets in the Field Sample Master File is based upon sample types. The table below describes these sample types, along with sub-groups within each sample type.

Sample Type Code (SAMPTYPE)	Description
HS	Original, randomly selected field sample. These sample results were to be used for the comparison analyses to determine if any differences in contamination levels existed between the Love Canal Emergency Declaration Area (EDA) and the comparison areas.

HS REP	Replacement field sample for an uncollectable original.
SPLIT	The field split half of a field sample was used to measure inter- and intra-laboratory variability. The field sample half retained the originally assigned project sample ID. The field split half was assigned a different project sample ID. Each of these halves contains a data element (PLSID) pointing to the other half.
FHB	Field handling blanks were "blind" Quality Control (QC) samples of uncontaminated soil used to measure whether cross-contamination had occurred.
PHB	Preparation handling blanks and PHB splits were QC samples sent to the analytic laboratories along with the field samples. They were not "blind" to the analysis laboratory and were not analyzed unless some contamination was measured in the field handling blanks.
HT	Holding time samples were soil samples used to study the effects of extending the sample holding time on LCIC concentration.

The first two sample types, "HS" and "HS REP," compose the group of field samples used for comparison purposes. For most purposes they are treated as a single group. Within the field sample group there are several sub-groups, including:

Sub-group	Description	Selection Logic
Samples not collected	Locations at which field samples were planned, but never were collected.	(SITENBR not = 0 and HSID = blanks)
Samples not prepared	Some of the field samples taken were not extrudable, and no replacements were able to be taken. These samples have neither preparation data nor analysis data.	(SAMPTYPE="HS" or "HS REP") and FSFCDTE > 0 and FSPMDTE = 0
Samples not analyzed	Some of the field samples that were prepared but could not be analyzed. These samples have no analysis data.	(SAMPTYPE="HS" or "HS REP") and FSFCDTE > 0 and FSPMDTE > 0 and FSAADTE = 0

Analyzed Field Samples	The field samples that were analyzed. Note that there are duplicate analyses present for some samples.	(SAMPTYPE="HS" or "HS REP") and FSAADTE > 0
Field Samples in Comparison Analysis	These were the field sample results (numbering 781) used in the statistical analyses.	Same as above plus the deletion of the 18 duplicates. See Section 8.6 for the list.

When working with the analyzed field samples, it should be noted that each sample was analyzed for the presence of eight analytes, the LCICs. Any use of the concentration results in FSFILE requires that the associated FORM1 file record (see Section 8) be merged to obtain the data usability flags associated with the results. Each analyte has its own data usability flag (LCICUSE1-LCICUSE8), and the usability of each analyte should be examined separately. For a description of the meaning of the usability flags, refer to the field descriptions in Section 2.3. Careful consideration should be exercised before using data not flagged as "GOOD." Refer to Volume III, Soil Assessment--Indicator Chemicals, Appendix H, CH2M HILL, 1988, for a complete explanation of the validation flags associated with a usability flag of "UNCERTAIN" or "BAD."

2.3 Data Element Dictionaries

The data element dictionaries for the Field Sample Master File and the Field Sample Ancillary File follow this page.

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FIELD SAMPLE MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
****** Keys and Status ******						
FS.A01	ALANALID		CHAR	23	Analysis Lab Sample Id (Lab Id + Lab Analysis Id)	LabData
FS.A02	FSSTATUS		CHAR	1	Status Flag Values: E = Validation Audit Failure blank = passed Validation Audit	IntDBBld
******* Inter-File Links/Secondary Keys *******						
FS.B01	ICANALID		CHAR	23	Initial Calibration Id (Lab Id + Lab Analysis Id of IC1)	LabData
FS.B02	CCANALID		CHAR	23	Continuing Calibration/Performance Check Id (Lab Id + Lab Analysis Id of CC/PC1)	LabData
FS.B03	MSANALID		CHAR	23	Matrix Spike Id (Lab Id + Lab Analysis Id)	LabData
FS.B04	MDANALID		CHAR	23	Matrix Spike Duplicate Id (Lab Id + Lab Analysis Id)	LabData
FS.B05	MBANALID		CHAR	23	Lab Method Blank Id (Lab Id + Lab Analysis Id)	LabData
FS.B06	RBANALID		CHAR	23	Reagent Blank Id (Lab Id + Lab Analysis Id)	LabData
FS.B07	QCANALID		CHAR	23	Quality Control Id (Lab Id + Lab Analysis Id) not currently used	
FS.B08	CLEANHS		CHAR	8	Original Project Id (HS Number)	IntDBBld
******* Intra-File Links/Secondary Keys *******						
FS.C01	HSID		CHAR	6	Project Field Sample Id (HS #)	SampTrac
FS.C02	FDUPID		CHAR	6	Revised Site Id (of the form nnnn or nnnnR); if no R suffix, resampling not done	SampTrac
FS.C03	FHBID		CHAR	6	Field Handling Blank Id (HS #)	SampTrac
FS.C04	SSBIDF		CHAR	6	Field Group Ship/Store Blank Id (HS #)	SampTrac
FS.C05	SSBIDP		CHAR	6	Prep Group Ship/Store Blank Id (HS #)	SampTrac
FS.C06	PHBID		CHAR	6	Prep Lab Handling Blank Id (HS #)	SampTrac
FS.C07	PLSID		CHAR	6	Prep Lab Split Id (HS #)	SampTrac
******* Chronology *******						
FS.D01	FSFCDTE		NUM	8	Field Collection Date	SampTrac
FS.D02	FSFCTME		NUM	8	Field Collection Time	SampTrac
FS.D03	FSFSDTE		NUM	8	Field Ship Date	SampTrac
FS.D04	FSPLDTE		NUM	8	Prep Lab Login Date	SampTrac
FS.D05	FSPMDTE		NUM	8	Prep Lab Mix Date	SampTrac
FS.D06	FSPMTME		NUM	8	Prep Lab Mix Time	SampTrac
FS.D07	FSPSDTE		NUM	8	Prep Lab Ship Date	SampTrac
FS.D08	FSALDTES		NUM	8	Analysis Lab Login Date (Sample Tracking)	SampTrac
FS.D09	FSALDTEL		NUM	8	Analysis Lab Login Date (LabData)	LabData
FS.D10	FSAEDTE		NUM	8	Analysis Lab Extract Date	LabData
FS.D11	FSAADTE		NUM	8	Analysis Lab Analysis Date	LabData
FS.D12	FSAATME		NUM	8	Analysis Lab Analysis Time	LabData
FS.D13	FSDBDTE		NUM	8	Data Validation Date	DataVal

LOVE CANAL HABITABILITY STUDY
FIELD SAMPLE MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
******* Data Transfer Tracking **********						
FS.E01	FSGENDTE		NUM	8	LabData Gen Date	LabData
FS.E02	FSGENTME		NUM	8	LabData Gen Time	LabData
FS.E03	FSADDDTE		NUM	8	DB Add Date	IntDBBld
FS.E04	FSADDTME		NUM	8	DB Add Time	IntDBBld
FS.E05	FSUPDDTE		NUM	8	DB Most Recent Update Date	IntDBBld
FS.E06	FSUPDTME		NUM	8	DB Most Recent Update Time	IntDBBld
FS.E07	FSUPDCNT		NUM	8	DB Update Count	IntDBBld
******* Field Sampling Data **********						
FS.F01	COLFORM		CHAR	5	Sample Collection Form #	SampTrac
FS.F02	COLFORMR		CHAR	5	Sample Collection Replacement Form #	SampTrac
FS.F03	SAMPTYPE		CHAR	6	Sample Type Values: 'HS ' = Field Sample 'HS REP' = Replacement Field Sample 'SPLIT' = Field Sample Split 'FHB' = Field Handling Blank 'SSB' = Shipping & Storage Blank 'SSB SP' = SSB Split 'PHB' = Prep Lab Handling Blank 'HT ' = Holding Time Blank 'UNK' = Unable to classify, no Project Id assigned	SampTrac
FS.F04	SITENBR		CHAR	4	Site Number	SampTrac
FS.F05	STREET		CHAR	70	Street Address	SampTrac
FS.F06	MEDIA		CHAR	1	Media (a constant of 'S')	SampTrac
FS.F07	XCOORD		NUM	8	Site X Coordinate	SampTrac
FS.F08	YCOORD		NUM	8	Site Y Coordinate	SampTrac
FS.F09	XACTUAL		NUM	8	Site X Coordinate	SampTrac
FS.F10	YACTUAL		NUM	8	Site Y Coordinate	SampTrac
FS.F11	LOCDIFF		NUM	8	Difference in feet between X/YCOORD & X/YACTUAL	SampTrac
FS.F12	AREAID		CHAR	1	Area Id Values: C = Cheektowaga E = EDA (Emergency Declaration Area I = Tonawanda N = Niagara Falls (CT221 and CT225) blank = no area (holding time blanks)	IntDBBld
FS.F13	NEIGHID		CHAR	2	Neighborhood Id	SampTrac
FS.F14	TEAMNBR		CHAR	2	Sampling Team Number	SampTrac
FS.F15	COLLECTR		CHAR	20	Sample Collector Name (text)	SampTrac
FS.F16	SOILCOMP		CHAR	80	Soil Composition	SampTrac
FS.F17	TUBENBR		CHAR	4	Collection Tube Number	SampTrac
FS.F18	COLMLEN		NUM	8	Length of Soil Column	SampTrac
FS.F19	DUPLICAT		CHAR	1	Duplicate Flag	currently not used
FS.F20	FLDCOM	(3)	CHAR	80	Field Comments (text 3X80)	SampTrac

LOVE CANAL HABITABILITY STUDY
FIELD SAMPLE MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
FS.F21	FCOCFORM		CHAR	4	Field Chain of Custody Form # (of the form Fnnn)	SampTrac
FS.F22	FTRFFORM		CHAR	4	Traffic Report for Tubes Form # (of the form nnnn)	SampTrac
FS.F23	FLFEDEX		CHAR	10	Fed Ex Airbill Number	SampTrac
FS.F24	FLSRMKS		CHAR	80	Field Shipping Special Instructions Field QC Samples Only Data	SampTrac
FS.F25	FLPRVBLK		CHAR	6	Previous Field Blank Id (HS #)	currently not used
******* Preparation Lab Data **********						
FS.G01	PREPLAB		CHAR	3	Prep Lab Id (a constant of 'CAA')	SampTrac
FS.G02	PREPCOND		CHAR	30	Condition on Receipt by Prep Lab (text)	SampTrac
FS.G03	PREPCOMM		CHAR	12	Sampling Team Comment	SampTrac
FS.G04	PLRECBY		CHAR	20	Person Receiving in Prep Lab	SampTrac
FS.G05	SPFORM		CHAR	5	Sample Preparation Form # (of the form Cnnnn)	SampTrac
FS.G06	MIXRNAME		CHAR	20	Mixer Name (text)	SampTrac
FS.G07	MIXTEAM		CHAR	1	Mixing Team Values: 1 = Team 1 2 = Team 2 3 = Team 3 blank = unknown	SampTrac
FS.G08	PREPCOM	(2)	CHAR	80	Prep Comments (text 2X80)	SampTrac
FS.G09	TRAKCOM		CHAR	19	Tracking Comment	SampTrac
FS.G10	SPLIT		CHAR	1	Designated Split Values: X = sample has been split; Id of split is contained in field PLSID blank = sample has not been split	SampTrac
FS.G11	PCOCFORM		CHAR	5	Prep Lab Chain of Custody Form # (of the form 'Ennn ')	SampTrac
FS.G12	PTRFFORM		CHAR	5	Traffic Report for Prepared Samples Form # (of the form 'Dnnn ')	SampTrac
FS.G13	MSFLAG		CHAR	1	Matrix Spike Flag	currently not used
FS.G14	PLJARNBR		NUM	8	Preparation Lab Jar Number	SampTrac
FS.G15	PLSPACE		NUM	8	Head Space	SampTrac
FS.G16	PLPOSHI		CHAR	1	Possible High Analysis Values Values: X = possible high concentration, subject to screening analysis prior to GC/MS blank = no screening analysis planned	SampTrac
FS.G17	PLSHMETH		CHAR	7	Preparation Lab Shipping Method (a constant of 'FED EX')	SampTrac
FS.G18	PLFEDEX		CHAR	10	Fed Ex Airbill Number	SampTrac
FS.G19	PLSRMKS		CHAR	80	Prep Lab Special Shipping Instructions Prep Lab QC Samples Only	SampTrac
FS.G20	PLPRVBLK		CHAR	6	Previous Prep Lab Blank Id (HS #)	currently not used

LOVE CANAL HABITABILITY STUDY
FIELD SAMPLE MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
FS.G21	EXCPFLAG		NUM	8	Exception Flag Values: 0 = sent to analysis lab 1 = collected, but not prepped 2 = prepped, sent to analysis lab, but only screened 3 = sample not collected	SampTrac
FS.G22	FTTEMP		NUM	8	Temperature inside cooler on arrival at preparation lab, in degrees Celsuis	SampTrac
FS.G23	TRTEMP		NUM	8	Temperature inside cooler on arrival at analytic lab, in degrees Celsuis	SampTrac
******* Analysis Lab Sample Login Data **********						
FS.H01	FSSMPL		CHAR	10	Project Sample Id	LabData
FS.H02	FSALID		CHAR	3	Analytic Laboratory Id Values: AQI CAA CEC EMS MGM NU2 = Contingency samples - for possible replacement; prepped and stored but never analyzed NUS VER blanks = no analysis performed; therefore no Lab Id	SampTrac
FS.H03	FSALCOND		CHAR	30	Condition on Receipt by Analysis Lab (text)	SampTrac
FS.H04	ALRECBY		CHAR	20	Person Receiving in Analysis Lab	SampTrac
FS.H05	FSRERUN		CHAR	2	Re-run Flag	currently not used
FS.H06	FSRRSTAT		CHAR	1	Re-run Type	currently not used
FS.H07	FSORIG		CHAR	1	Orig. Found Flag	currently not used
******* Analysis Lab Sample Extraction Data **********						
FS.I01	FSTWTEXT		NUM	8	Target Weight to Extract (gm)	LabData
FS.I02	FSWTEXT		NUM	8	Weight Extracted (gm)	LabData
FS.I03	FSMOIST		NUM	8	Percent Moisture	LabData
FS.I04	FSCONCDF		NUM	8	Concentration Dilution Factor	LabData
FS.I05	FSEXTANL		CHAR	8	Extraction Analyst	LabData

LOVE CANAL HABITABILITY STUDY
FIELD SAMPLE MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
******* Analysis Lab Injection Data **********						
FS.J01	FSINSTID		CHAR	15	GC/MS Instrument Id	LabData
FS.J02	FSANLST		CHAR	8	GC/MS Analyst	LabData
FS.J03	FSFILE		CHAR	15	GC/MS Datafile Id	LabData
FS.J04	FSINJVOL		NUM	8	Injection Volume (ul)	LabData
******* Analysis Lab Interpretation Data **********						
FS.K01	FSQFILE		CHAR	12	GC/MS Shift Results File Name	LabData
FS.K02	FSQMTH	(8,3)	CHAR	1	Quantitation Method Flag, by 8 LCICs, by 3 Ions Values: blank) or) = GC/MS Automatic Area Quantitation A) H = Peak Height Quantitation M = GC/MS Manual Quantitation O = Computed using area by LabData with correction data	LabData
FS.K03	FSQION	(8)	CHAR	1	LCIC Quantitation Ion Selection, by 8 LCICs Values: blank = primary ion used for quantitation S = secondary ion used for quantitation T = tertiary ion used for quantitation	LabData
FS.K04	FSLCPH	(8,3)	NUM	8	Peak Height, by 8 LCICs, by 3 Ions	LabData
FS.K05	FSISPH	(5)	NUM	8	Peak Height, by 5 Int. Stds. (Primary Ion)	LabData
FS.K06	FSPYRPH		NUM	8	Peak Height Pyrene-D10 (Secondary Ion)	LabData
FS.K07	FSSSPH	(3)	NUM	8	Peak Height, by 3 Surrogates (Primary Ion)	LabData
FS.K08	FSHLCS	(8,3)	NUM	8	Scan for Peak Height, by 8 LCICs, by 3 Ions	LabData
FS.K09	FSHLCR	(8,3)	NUM	8	Retention Time for Peak Height, by 8 LCICs, by 3 Ions	LabData
FS.K10	FSHISS	(5)	NUM	8	Scan for Peak Height, by 5 Int. Stds.	LabData
FS.K11	FSHISR	(5)	NUM	8	Retention Time for Peak Height, by 5 Int. Stds.	LabData
FS.K12	FSHPYRS		NUM	8	Scan for Peak Height for Pyrene-D10	LabData
FS.K13	FSHPYRR		NUM	8	Retention Time for Peak Height for Pyrene-D10	LabData
FS.K14	FSHSSS	(3)	NUM	8	Scan for Peak Height, by 3 Surrogates	LabData
FS.K15	FSHSSR	(3)	NUM	8	Retention Time for Peak Height, by 3 Surrogates	LabData
******* Correction Flags ********** Values: Y = data corrected, original data stored in ancillary file blank = data not corrected, no data stored in ancillary file						
FS.L01	FSCDATE		CHAR	1	Analysis Lab Analysis Date	LabData
FS.L02	FSCTIME		CHAR	1	Analysis Lab Analysis Time	LabData
FS.L03	FSCANAL		CHAR	1	Analyst Entering the Correction Data	LabData
FS.L04	FSCLCA	(8,3)	CHAR	1	Area, by 8 LCICs, by 3 Ions	LabData
FS.L05	FSCLCS	(8,3)	CHAR	1	Scan, by 8 LCICs, by 3 Ions	LabData
FS.L06	FSCLCR	(8,3)	CHAR	1	Retention Time, by 8 LCICs, by 3 Ions	LabData
FS.L07	FSCISA	(5)	CHAR	1	Area, by 5 Int. Stds. (Primary Ion)	LabData

LOVE CANAL HABITABILITY STUDY
FIELD SAMPLE MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
FS.L08	FSCISS	(5)	CHAR	1	Scan, by 5 Int. Stds. (Primary Ion)	LabData
FS.L09	FSCISR	(5)	CHAR	1	Retention Time, by 5 Int. Stds. (Primary Ion)	LabData
FS.L10	FSCPYRA		CHAR	1	Area Pyrene-D10 (Secondary Ion)	LabData
FS.L11	FSCPYRS		CHAR	1	Scan Pyrene-D10 (Secondary Ion)	LabData
FS.L12	FSCPYRR		CHAR	1	Retention Time Pyrene-D10 (Secondary Ion)	LabData
FS.L13	FSCSSA	(3)	CHAR	1	Area, by 3 Surrogates (Primary Ion)	LabData
FS.L14	FSCSSS	(3)	CHAR	1	Scan, by 3 Surrogates (Primary Ion)	LabData
FS.L15	FSCSSR	(3)	CHAR	1	Retention Time, by 3 Surrogates (Primary Ion)	LabData
******* Analysis Raw Data (After Corrections, if any) **********						
FS.M01	FSLCA	(8,3)	NUM	8	Area, by 8 LCICs, by 3 Ions	LabData
FS.M02	FSLCS	(8,3)	NUM	8	Scan, by 8 LCICs, by 3 Ions	LabData
FS.M03	FSLCR	(8,3)	NUM	8	Retention Time, by 8 LCICs, by 3 Ions	LabData
FS.M04	FSISA	(5)	NUM	8	Area, by 5 Int. Stds. (Primary Ion)	LabData
FS.M05	FSPYRA		NUM	8	Area Pyrene-D10 (Secondary Ion)	LabData
FS.M06	FSISS	(5)	NUM	8	Scan, by 5 Int. Stds. (Primary Ion)	LabData
FS.M07	FSPYRS		NUM	8	Scan Pyrene-D10 (Secondary Ion)	LabData
FS.M08	FSISR	(5)	NUM	8	Retention Time, by 5 Int. Stds. (Primary Ion)	LabData
FS.M09	FSPYRR		NUM	8	Retention Time Pyrene-D10 (Secondary Ion)	LabData
FS.M10	FSSSA	(3)	NUM	8	Area, by 3 Surrogates (Primary Ion)	LabData
FS.M11	FSSSS	(3)	NUM	8	Scan, by 3 Surrogates (Primary Ion)	LabData
FS.M12	FSSSR	(3)	NUM	8	Retention Time, by 3 Surrogates (Primary Ion)	LabData
******* LabData Computations for Field Samples **********						
FS.N01	FSRR	(8)	NUM	8	Relative Retention Time, by 8 LCICs (Quantitation Ion)	*LabData
FS.N02	FSRRC	(8)	NUM	8	Relative Retention Time Criteria, by 8 LCICs	LabData
FS.N03	FSRRF	(8)	CHAR	1	Flag for Rel. Ret. Time Out of Criteria, by 8 LCICs Values: * = Out of criteria blank = Within criteria	*LabData
FS.N04	FSCONCB	(8)	NUM	8	PreID-criteria Concentration, by 8 LCICs (i.e. primary ion equivalent concentration)	*LabData
FS.N05	FSCONCA	(8)	NUM	8	Id Criteria applied Concentration, by 8 LCICs	*LabData
FS.N06	FSIRAT	(8)	NUM	8	Ion Ratio, by 8 LCICs	*LabData
FS.N07	FSIONF	(8)	CHAR	1	Flag for All Ions Being Present, by 8 LCICs Values: * = All ions present blank = One or more ions not present	*LabData
FS.N08	FSMINS	(8)	NUM	8	Minimum Scan Number of 3 Ions, by 8 LCICs	LabData
FS.N09	FSMAXS	(8)	NUM	8	Maximum Scan Number of 3 Ions, by 8 LCICs	LabData
FS.N10	FSRANG	(8)	NUM	8	Scan Range (Max - Min), by 8 LCICs	*LabData
FS.N11	FSRANGF	(8)	CHAR	1	Flag for Scan range > 2, by 8 LCICs Values: * = Scan range greater than 2 blank = Scan range not greater than 2	*LabData
FS.N12	FSIDEVT	(8)	NUM	8	Ion Ratio % Dev. from Theoretical Values, by 8 LCICs	*LabData

LOVE CANAL HABITABILITY STUDY
FIELD SAMPLE MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENG.H	DESCRIPTION	SOURCE
FS.N13	FSIDEVF	(8)	CHAR	1	Flag for Ion ratio % Dev. Out of Criteria, by 8 LCICs Values: * = Ion ratio out of criteria; greater than 40% + = Ion ratio out of criteria; 20% < ratio <= 40% blank = Ion ratio within criteria	*LabData
FS.N14	FSPRESCR		CHAR	3	Flag for Analysis Pre-screen Values: 'MS ' = GC/MS pre-screening performed 'ECD' = GC/ECD pre-screening performed blanks = no pre-screening done	LabData
FS.N15	FSSULFUR		CHAR	1	Flag for Sulphur Cleanup Performed Values: Y = sulphur cleanup performed blank or N = no sulphur cleanup performed	LabData
******* LabData Computations for Surrogate Standards **********						
FS.001	FSPR	(3)	NUM	8	% Recovery by 3 Surrogates	*LabData
FS.002	FSPRF	(3)	CHAR	1	Flag for % Rec. Out of Criteria, by 3 Surrogates Values: * = Out of criteria blank = Within criteria	*LabData
FS.003	FSSSADD	(3)	NUM	8	Amount of Surrogate added(ng), by 3 Surrogates	LabData
FS.004	FSPRCL	(3)	NUM	8	% Recovery Criteria lower limit, by 3 Surrogates	LabData
FS.005	FSPRCU	(3)	NUM	8	% Recovery Criteria upper limit, by 3 Surrogates	LabData
FS.006	FSPROUT		NUM	8	Number of % Rec. Out of Criteria	LabData
******* LabData Computations for Internal Standards **********						
FS.P01	FSISADD		NUM	8	Internal Standard Quantity Added (in nanograms)	LabData
FS.P02	FSRD	(5)	NUM	8	Ret. Time Difference From CC Val, by 5 Int Stds	*LabData
FS.P03	FSAD	(5)	NUM	8	Area Difference % From CC Val, by 5 Int Stds	*LabData
FS.P04	FSRF	(5)	CHAR	1	Flag for Ret. Time Out of Criteria, by 5 Int Stds Values: * = Out of criteria blank = Within criteria	*LabData
FS.P05	FSAF	(5)	CHAR	1	Flag for Area Out of Criteria, by 5 Int Stds Values: * = Out of criteria blank = Within criteria	*LabData
FS.P06	FSRDC	(5)	NUM	8	Retention Time Difference Criteria, by 5 Int Stds	LabData
FS.P07	FSADCL	(5)	NUM	8	Area % Diff. Crit. lower limit, by 5 Int Stds	LabData
FS.P08	FSADCU	(5)	NUM	8	Area % Diff. Crit. upper limit, by 5 Int Stds	LabData

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FIELD SAMPLE MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
******* Data Validation Flags and Comments **********						
	Values: (not currently available)					
FS.Q01	FSSURRA		CHAR	1	Check surrogates spiked in all samples	DataVal
FS.Q02	FSSURRB		CHAR	1	Surrogates recoveries within criteria	DataVal
FS.Q03	FSSURRC		CHAR	1	Surrogates Miscellaneous	DataVal
FS.Q04	FSSURCM	(3)	CHAR	60	Surrogates Comments	DataVal
FS.Q05	FSINTA		CHAR	1	Internal Standards RT Criteria	DataVal
FS.Q06	FSINTB		CHAR	1	Internal Standards Area Criteria	DataVal
FS.Q07	FSINTC		CHAR	2	Internal Standards Miscellaneous	DataVal
FS.Q08	FSINTCM	(3)	CHAR	60	Internal Standards Comments	DataVal
FS.Q09	FSIDA		CHAR	1	Id All ions maximize simultaneously	DataVal
FS.Q10	FSIDB		CHAR	1	Id Appropriate flags used.	DataVal
FS.Q11	FSIDC		CHAR	1	Id All peaks reported that meet id criteria	DataVal
FS.Q12	FSIDD		CHAR	2	Id Low level peaks examined	DataVal
FS.Q13	FSIDE		NUM	2	Id Miscellaneous	DataVal
FS.Q14	FSIDCOM	(3)	CHAR	60	Id Comments	DataVal
FS.Q15	FSQTA		CHAR	1	Quantitation appropriate RRF's used if nonstandard	DataVal
FS.Q16	FSQTB		CHAR	1	Check integration parameters if manual quant. used	DataVal
FS.Q17	FSQTC		CHAR	2	Quantitation Miscellaneous	DataVal
FS.Q18	FSQTCOM	(3)	CHAR	60	Quantitation Comments	DataVal
FS.Q19	FSGENA		CHAR	2	Review case narrative and address all problems	DataVal
FS.Q20	FSGENB		CHAR	2	Examine SICPS	DataVal
FS.Q21	FSGENC		CHAR	2	Examine quantitation reports	DataVal
FS.Q22	FSGEND		CHAR	2	General Miscellaneous	DataVal
FS.Q23	FSGENCM	(3)	CHAR	60	General Comments	DataVal
FS.Q24	FSDQ	(8,5)	CHAR	2	Data Qualifier flags samples by analyte	DataVal
******* Integrated DB Audit System Flags **********						
	Values (except where indicated otherwise):					
	blank = record found / no discrepancy / no difference					
	'*' = record not found / discrepancy / difference					
FS.R01	FSTRACK		CHAR	1	Flag for Sample NOT Found in Sample Tracking	IntDBBld
FS.R02	FSF1FLAG		CHAR	1	Flag for Sample Match to FORM1 Master File	IntDBBld
					Values:	
					1 = Found FORM1 and All data matches	
					2 = Found FORM1 and some data does not match	
					3 = No FORM1 found	
					blank = FORM1 match not attempted (sample tracking records not matching field sample records)	
FS.R03	FSICREF		CHAR	1	Flag for IC not found or date/time inconsistent	IntDBBld
FS.R04	FSCCREF		CHAR	1	Flag for CC not found or date/time inconsistent	IntDBBld
FS.R05	FSMSREF		CHAR	1	Flag for MS not found	IntDBBld
FS.R06	FSMDREF		CHAR	1	Flag for MSD not found	IntDBBld
FS.R07	FSRBREF		CHAR	1	Flag for RB not found	IntDBBld
FS.R08	FSMBREF		CHAR	1	Flag for MB not found	IntDBBld
FS.R09	FSDUP		CHAR	1	Flag for Field Duplicate not found	currently not used
FS.R10	FSFHB		CHAR	1	Flag for Field Handling Blank not found	currently not used

LOVE CANAL HABITABILITY STUDY
FIELD SAMPLE MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
FS.R11	FSSSBF		CHAR	1	Flag for Shipping & Storage Blank not found	currently not used
FS.R12	FSSSBP		CHAR	1	Flag for Shipping & Storage Blank not found	currently not used
FS.R13	FSPHB		CHAR	1	Flag for Prep Lab Handling Blank not found	currently not used
FS.R14	FSPLS		CHAR	1	Flag for Prep Lab Split not found	currently not used
FS.R15	FSRECALC		CHAR	1	Flag for recalculation discrepancy on at least one data element computed by LabData system (within .2% tolerance)	IntDBBld
FS.R16	FSDIFLAB		CHAR	1	Flag for diff. lab between LabData & Samptrac	currently not used

LOVE CANAL HABITABILITY STUDY

FIELD SAMPLE ANCILLARY FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
****** Keys ******						
FA.A01	ALANALID		CHAR	23	Analysis Lab Sample Id (Lab Id + Lab Analysis Id)	LabData
******* Data Transfer Tracking *******						
FA.B01	FSGENDTE		NUM	8	LabData Gen Date	LabData
FA.B02	FSGENTME		NUM	8	LabData Gen Time	LabData
FA.B03	FSADDDTE		NUM	8	DB Add Date	IntDBBld
FA.B04	FSADDTME		NUM	8	DB Add Time	IntDBBld
FA.B05	FSUPDDTE		NUM	8	DB Most Recent Update Date	IntDBBld
FA.B06	FSUPDTME		NUM	8	DB Most Recent Update Time	IntDBBld
FA.B07	FSUPDCNT		NUM	8	DB Update Count	IntDBBld
******* Data Replaced by Corrections *******						
FA.C01	FSLCA	(8,3)	NUM	8	Area, by 8 LCICs, by 3 Ions	LabData
FA.C02	FSLCS	(8,3)	NUM	8	Scan, by 8 LCICs, by 3 Ions	LabData
FA.C03	FSLCR	(8,3)	NUM	8	Retention Time, by 8 LCICs, by 3 Ions	LabData
FA.C04	FSISA	(5)	NUM	8	Area, by 5 Int. Stds. (Primary Ion)	LabData
FA.C05	FSPYRA		NUM	8	Area Pyrene-D10 (Secondary Ion)	LabData
FA.C06	FSISS	(5)	NUM	8	Scan, by 5 Int. Stds. (Primary Ion)	LabData
FA.C07	FSPYRS		NUM	8	Scan Pyrene-D10 (Secondary Ion)	LabData
FA.C08	FSISR	(5)	NUM	8	Retention Time, by 5 Int. Stds. (Primary Ion)	LabData
FA.C09	FSPYRR		NUM	8	Retention Time Pyrene-D10 (Secondary Ion)	LabData
FA.C10	FSSSA	(3)	NUM	8	Area, by 3 Surrogates (Primary Ion)	LabData
FA.C11	FSSSS	(3)	NUM	8	Scan, by 3 Surrogates (Primary Ion)	LabData
FA.C12	FSSSR	(3)	NUM	8	Retention Time, by 3 Surrogates (Primary Ion)	LabData

3.0 Initial Calibration Master File and Ancillary File

In the Initial Calibration Master File, a record contains all quantitation report and computed data for each five-point initial calibration and/or EPA performance check analysis run on the GC/MS. The performance check analysis could be run either in the same analytic run (i.e., "shift") as the five-point, or in a later shift. Therefore some records contain the five-point data and the performance check data; some records, only the five-point data; and some records, only the performance check data. Logically, this data represents the top of the data structure. All continuing calibrations are associated with a five-point initial calibration; thus one or many continuing calibration records will point to a single initial calibration record.

3.1 Logical Record Description

A logical record in this file contains data for one five-point initial calibration and/or EPA performance check. The data elements are organized in groups, as follows:

- KEYS AND STATUS - the primary, unique identifier of each record in the file, along with any other (perhaps non-unique) keys, and the status flag.

- CHRONOLOGY - dates and times of significant events during the processing of the sample.

- DATA TRANSFER TRACKING - system dates used for maintenance of the data base.

- ANALYSIS LAB SAMPLE LOGIN DATA - data entered by the analytic laboratory when the sample was logged into their facility.

- ANALYSIS LAB INJECTION DATA - data entered by the lab relating to injection of the sample in the GC/MS.

- ANALYSIS LAB INTERPRETATION DATA - data identifying the shift results file that the sample belonged to, the quantitation method used for each analyte, and the ion used for quantitation for each analyte. This data also contains the results of the GC/MS analysis when the peak height method of quantitation was used.

- CORRECTION FLAGS - flags used to indicate whether or not a particular element has been corrected/updated. If a flag is set "on" ("Y"), then the updated data is contained in this file, and the original data value is stored in the ancillary file record.

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- ANALYSIS RAW DATA - (after corrections, if any) raw data generated by the GC/MS. This is essentially the same data contained on the quantitation report created by the GC/MS.

- LABDATA COMPUTATIONS FOR INITIAL CALIBRATION - results calculated by the LabData system using the raw data generated by the GC/MS. It includes the initial calibration response factor results, the QC criteria, and flags indicating whether or not the criteria were met.

- LABDATA COMPUTATIONS FOR EMSL PERFORMANCE CHECK - results calculated by the LabData system using the raw data generated by the GC/MS. It includes the initial calibration percent recovery results, the QC criteria, and flags indicating whether or not the criteria were met.

- DATA VALIDATION FLAGS AND COMMENTS - results of the data validation for the sample performed by EMSL-LV. It includes data validation checklist responses, comments, validation flags, and EMSL-LV usability flags.

- INTEGRATED DATA BASE AUDIT SYSTEM FLAGS - results of the automated audits and validations performed during the data base building process.

The ancillary file consists of three groups: KEYS, CHRONOLOGY, and DATA REPLACED BY CORRECTIONS. The last group corresponds to the ANALYSIS RAW DATA group in terms of data elements, but contains original data that has been replaced in the master file by corrected data.

3.2 Logical Subsets of the File - Special Screening

There are two primary groups of logical subsets in the Initial Calibration (IC) Master File. Initially, the design of the data base assumed that an EPA Performance Check Standard analysis would be analyzed in the same analytic run as the five-point initial calibration. Accordingly, a record in the IC file was designed to contain each five-point analysis and one EPA Performance Check. Unfortunately, this did not turn out to always be the case. In most cases, the EPA Performance Check was run with the five-point analysis, and the IC record contains all six analyses. In some cases, the EPA Performance Check was run in a later analysis shift and, as a result, is contained in a separate IC file record. Thus some IC file records have only the five-point analyses data, some have only the EPA Performance Check data, and some have both. Since the data are typically analyzed separately, this limitation should not be a problem.

To obtain those records containing five-point analyses, select those records where the field ICSMPL1 = "IC1". To obtain those records containing an EPA Performance Check, select those records where the field ICSMPL6 = "EMPC" in the first four character positions (in SAS use the SUBSTR command).

3.3 Data Element Dictionaries

The data element dictionaries for the Initial Calibration Master File and the Initial Calibration Ancillary File follow this page.

LOVE CANAL HABITABILITY STUDY

INITIAL CALIBRATION MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
***** Keys and Status *****						
IC.A01	ICANALID		CHAR	23	Initial Calibration Id (Lab Id + Lab Analysis Id of the IC1 analysis)	LabData
IC.A02	ICANAL	(4)	CHAR	23	Initial Calibration Id (Lab Id + Lab Analysis Id of the IC2-IC5 analyses)	LabData
IC.A03	ICSTATUS		CHAR	1	Status Flag Values: E = Validation Audit Failure blank = Passed Validation Audit	IntDBBld
******* Chronology *******						
IC.B01	ICAADTE	(6)	NUM	8	Analysis Lab Analysis Date, by 5 Calibration Concentrations and EMSL PC	LabData
IC.B02	ICAATME	(6)	NUM	8	Analysis Lab Analysis Time by 5 Calibration Concentrations and EMSL PC	LabData
******* Data Transfer Tracking *******						
IC.C01	ICGENDTE		NUM	8	LabData Gen Date	LabData
IC.C02	ICGENTME		NUM	8	LabData Gen Time	LabData
IC.C03	ICADDDTE		NUM	8	DB Add Date	IntDBBld
IC.C04	ICADDTME		NUM	8	DB Add Time	IntDBBld
IC.C05	ICUPDDTE		NUM	8	DB Most Recent Update Date	IntDBBld
IC.C06	ICUPDTME		NUM	8	DB Most Recent Update Time	IntDBBld
IC.C07	ICUPDCNT		NUM	8	DB Update Count	IntDBBld
******* Analysis Lab Sample Login Data *******						
IC.D01	ICSMPL	(6)	CHAR	10	Project Sample Id for IC1 thru IC5 and EMSL PC Values for each of ICSMPL1 through ICSMPL5: 'ICn ' = Initial calibration record generated by a five-point initial calibration (Where ICn takes the value of IC1 in ICSMPL1, IC2 in ICSMPL2, etc. through IC5) blank = Initial calibration record generated by a stand-alone EMSL performance check Values for ICSMPL6: blank = no EMSL performance check data in this record (only five-point calibration data) 'EMPC' in the first four positions = EMSL performance check data in this record	LabData

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INITIAL CALIBRATION MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
IC.D02	ICALID		CHAR	3	Analytic Laboratory Id Values: AQI CAA CEC EMS MGM NU2 = Contingency samples - for possible replacement; prepped and stored but never analyzed NUS VER blanks = no analysis performed; therefore no Lab Id	LabData
******* Analysis Lab Injection Data **********						
IC.E01	ICINSTID		CHAR	15	GC/MS Instrument Id	LabData
IC.E02	ICINSTMF		CHAR	20	GC/MS Instrument Manufacturer	LabData
IC.E03	ICINSTMN		CHAR	20	GC/MS Instrument Model Number	LabData
IC.E04	ICISCODE		CHAR	1	Internal Standard Solution Code	LabData
IC.E05	ICSOLCD	(5)	CHAR	1	Initial Calibration Solution Codes (5)	LabData
IC.E06	ICCCCODE		CHAR	1	Continuing Calibration Solution Code	LabData
IC.E07	ICCOLMMF		CHAR	20	Column Manufacturer	LabData
IC.E08	ICCOLMSN		CHAR	20	Column Serial Number	LabData
IC.E09	ICANLST	(6)	CHAR	8	Analyst, by 5 Calibration Concentrations and EMSL PC	LabData
IC.E10	ICFILE	(6)	CHAR	15	Datafile Id, by 5 Calibration Concentrations and EMSL PC	LabData
IC.E11	ICINJVL	(6)	NUM	8	Injection Volume (ul), by 5 Calibration Concentrations and EMSL PC	LabData
******* Analysis Lab Interpretation Data **********						
IC.F01	ICQFILE		CHAR	12	GC/MS Shift Results File Name For IC2 ONLY:	LabData
IC.F02	ICQMTH	(8,3)	CHAR	1	Quantitation Method Flag, by 8 LCICs, by 3 Ions Values: blank) or) = GC/MS Automatic Area Quantitation A) H = Peak Height Quantitation M = GC/MS Manual Quantitation O = Computed using area by LabData with correction data	LabData
IC.F03	ICQION	(8)	CHAR	1	LCIC Quantitation Ion Selection, by 8 LCICs Values: blank = primary ion used for quantitation S = secondary ion used for quantitation	LabData

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INITIAL CALIBRATION MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
					T = tertiary ion used for quantitation	
IC.F04	ICLCPH	(8,3)	NUM	8	Peak Height, by 8 LCICs, by 3 Ions	LabData
IC.F05	ICISPH	(5)	NUM	8	Peak Height, by 5 Int. Stds. (Primary Ion)	LabData
IC.F06	ICPYRPH		NUM	8	Peak Height Pyrene-D10 (Secondary Ion)	LabData
IC.F07	ICSSPH	(3)	NUM	8	Peak Height, by 3 Surrogates (Primary Ion)	LabData
IC.F08	ICHLCS	(8,3)	NUM	8	Scan for Peak Height, by 8 LCICs, by 3 Ions	LabData
IC.F09	ICHLCR	(8,3)	NUM	8	Retention Time for Peak Height, by 8 LCICs, by 3 Ions	LabData
IC.F10	ICHISS	(5)	NUM	8	Scan for Peak Height, by 5 Int. Stds.	LabData
IC.F11	ICHISR	(5)	NUM	8	Retention Time for Peak Height, by 5 Int. Stds.	LabData
IC.F12	ICHPYRS		NUM	8	Scan for Peak Height for Pyrene-D10	LabData
IC.F13	ICHPYRR		NUM	8	Retention Time for Peak Height for Pyrene-D10	LabData
IC.F14	ICHSSS	(3)	NUM	8	Scan for Peak Height, by 3 Surrogates	LabData
IC.F15	ICHSSR	(3)	NUM	8	Retention Time for Peak Height, by 3 Surrogates	LabData
******* Correction Flags (For IC2 ONLY) **********						
					Values:	
					Y = data corrected, original data stored in ancillary file	
					blank = data not corrected, no data stored in ancillary file	
IC.G01	ICCDATE		CHAR	1	Analysis Lab Analysis Date	LabData
IC.G02	ICCTIME		CHAR	1	Analysis Lab Analysis Time	LabData
IC.G03	ICCANAL		CHAR	1	Analyst	LabData
IC.G04	ICCLCA	(8,3)	CHAR	1	Area, by 8 LCICs, by 3 Ions	LabData
IC.G05	ICCLCS	(8,3)	CHAR	1	Scan, by 8 LCICs, by 3 Ions	LabData
IC.G06	ICCLCR	(8,3)	CHAR	1	Retention Time, by 8 LCICs, by 3 Ions	LabData
IC.G07	ICCISA	(5)	CHAR	1	Area, by 5 Int. Stds. (Primary Ion)	LabData
IC.G08	ICCISS	(5)	CHAR	1	Scan, by 5 Int. Stds. (Primary Ion)	LabData
IC.G09	ICCISR	(5)	CHAR	1	Retention Time, by 5 Int. Stds. (Primary Ion)	LabData
IC.G10	ICCPYRA		CHAR	1	Area Pyrene-D10 (Secondary Ion)	LabData
IC.G11	ICCPYRS		CHAR	1	Scan Pyrene-D10 (Secondary Ion)	LabData
IC.G12	ICCPYRR		CHAR	1	Retention Time Pyrene-D10 (Secondary Ion)	LabData
IC.G13	ICCSSA	(3)	CHAR	1	Area, by 3 Surrogates (Primary Ion)	LabData
IC.G14	ICCSSS	(3)	CHAR	1	Scan, by 3 Surrogates (Primary Ion)	LabData
IC.G15	ICCSSR	(3)	CHAR	1	Retention Time, by 3 Surrogates (Primary Ion)	LabData
******* Analysis Raw Data, By 5 Calibration Concentrations and EMSL Performance Check**********						
					(After Corrections, if any)	
IC.H01	ICLCA	(6,8,3)	NUM	8	Area, by 8 LCICs, by 3 Ions	LabData
IC.H02	ICLCS	(6,8,3)	NUM	8	Scan, by 8 LCICs, by 3 Ions	LabData
IC.H03	ICLCR	(6,8,3)	NUM	8	Retention Time, by 8 LCICs, by 3 Ions	LabData
IC.H04	ICISA	(6,5)	NUM	8	Area, by 5 Int. Stds. (Primary Ion)	LabData

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INITIAL CALIBRATION MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
IC.H05	ICPYRA	(6)	NUM	8	Area Pyrene-D10 (Secondary Ion)	LabData
IC.H06	ICISS	(6,5)	NUM	8	Scan, by 5 Int. Stds. (Primary Ion)	LabData
IC.H07	ICPYRS	(6)	NUM	8	Scan Pyrene-D10 (Secondary Ion)	LabData
IC.H08	ICISR	(6,5)	NUM	8	Retention Time, by 5 Int. Stds. (Primary Ion)	LabData
IC.H09	ICPYRR	(6)	NUM	8	Retention Time Pyrene-D10 (Secondary Ion)	LabData
IC.H10	ICSSA	(6,3)	NUM	8	Area, by 3 Surrogates (Primary Ion)	LabData
IC.H11	ICSSS	(6,3)	NUM	8	Scan, by 3 Surrogates (Primary Ion)	LabData
IC.H12	ICSSR	(6,3)	NUM	8	Retention Time, by 3 Surrogates (Primary Ion)	LabData
******* LabData Computations for Initial Calibration**********						
IC.I01	ICMRF	(11)	NUM	8	Mean Response Factors, by 8 LCICs and 3 Surrogates	*LabData
IC.I02	ICRSD	(11)	NUM	8	% Relative Std. Dev., by 8 LCICs and 3 Surrogates	*LabData
IC.I03	ICRSDC	(11)	NUM	8	% Relative Std. Dev. criteria, by 8 LCICs and 3 Surrogates	LabData
IC.I04	ICRSDF	(11)	CHAR	1	Flag for % Relative Std. Dev. out of criteria, by 8 LCICs and 3 Surrogates Values: * = Out of criterin blank = Within criteria	*LabData
IC.I05	ICRSDOUT		NUM	8	Number of % Relative Std. Dev. out of criteria	LabData
IC.I06	ICRF	(11,5)	NUM	8	Response Factors, by 8 LCICs and 3 surrogates, by 5 Calibration Concentrations	*LabData
IC.I07	ICCONC	(5)	NUM	8	Concentrations, by 5 Calibration Concentrations	LabData
******* LabData Computations for EMSL Performance Check **********						
IC.J01	PCTCON	(11)	NUM	8	Theoretical Concentrations, by 8 LCICs and 3 Surrogates	LabData
IC.J02	PCPRLC	(11)	NUM	8	% Recovery Lower Criteria, by 8 LCICs and 3 Surrogates	LabData
IC.J03	PCPRUC	(11)	NUM	8	% Recovery Upper Criteria, by 8 LCICs and 3 Surrogates	LabData
IC.J04	PCPROUT		NUM	8	Number of % Recovery Out of Criteria	LabData
IC.J05	PCCONC	(11)	NUM	8	Concentrations, by 8 LCICs and 3 Surrogates	*LabData
IC.J06	PCPR	(11)	NUM	8	% Recovery, by 8 LCICs and 3 Surrogates	*LabData
IC.J07	PCPRF	(11)	CHAR	1	Flag for % Recovery Within Criteria, by 8 LCICs and 3 Surrogates Values: * = Out of criterin blank = Within criteria	*LabData
IC.J08	PCISADD		NUM	8	Amount of Internal Standard Added	LabData
IC.J09	PCVOLMCS		NUM	8	Volume of Check Standard Solution	LabData

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INITIAL CALIBRATION MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
******* Data Validation Flags and Comments **********						
Values: (currently not available)						
IC.K01	ICCALA		CHAR	1	IC % RSD exceptions checked	DataVal
IC.K02	ICCALB		CHAR	2	IC check quantitation reports for evidence of editing	DataVal
IC.K03	ICCALC		CHAR	2	IC examine chromatograms	DataVal
IC.K04	ICCALD		CHAR	2	IC Miscellaneous	DataVal
IC.K05	ICDVCOM	(3)	CHAR	60	IC Comments	DataVal
******* Integrated DB Audit System Results **********						
IC.L01	ICRECALC		CHAR	1	Flag for calculation discrepancies Values: * = Discrepancy (could be a result of not having all five-points plus performance check) blank = No discrepancy	IntDBBld

LOVE CANAL HABITABILITY STUDY

INITIAL CALIBRATION ANCILLARY FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
***** Keys *****						
IA.A01	ICANALID		CHAR	23	Initial Calibration Id (Lab Id + Lab Analysis Id of the IC1 analysis)	LabData
******* Data Transfer Tracking *******						
IA.B01	ICGENDTE		NUM	8	LabData Gen Date	LabData
IA.B02	ICGENTME		NUM	8	LabData Gen Time	LabData
IA.B03	ICADDDTE		NUM	8	DB Add Date	IntDBBld
IA.B04	ICADDTME		NUM	8	DB Add Time	IntDBBld
IA.B05	ICUPDDTE		NUM	8	DB Most Recent Update Date	IntDBBld
IA.B06	ICUPDTME		NUM	8	DB Most Recent Update Time	IntDBBld
IA.B07	ICUPDCNT		NUM	8	DB Update Count	IntDBBld
******* Data Replaced by Corrections *******						
IA.C01	ICLCA	(6,8,3)	NUM	8	Area, by 8 LCICs, by 3 Ions	LabData
IA.C02	ICLCS	(6,8,3)	NUM	8	Scan, by 8 LCICs, by 3 Ions	LabData
IA.C03	ICLCR	(6,8,3)	NUM	8	Retention Time, by 8 LCICs, by 3 Ions	LabData
IA.C04	ICISA	(6,5)	NUM	8	Area, by 5 Int. Stds. (Primary Ion)	LabData
IA.C05	ICPYRA	(6)	NUM	8	Area Pyrene-D10 (Secondary Ion)	LabData
IA.C06	ICISS	(6,5)	NUM	8	Scan, by 5 Int. Stds. (Primary Ion)	LabData
IA.C07	ICPYRS	(6)	NUM	8	Scan Pyrene-D10 (Secondary Ion)	LabData
IA.C08	ICISR	(6,5)	NUM	8	Retention Time, by 5 Int. Stds. (Primary Ion)	LabData
IA.C09	ICPYRR	(6)	NUM	8	Retention Time Pyrene-D10 (Secondary Ion)	LabData
IA.C10	ICSSA	(6,3)	NUM	8	Area, by 3 Surrogates (Primary Ion)	LabData
IA.C11	ICSSS	(6,3)	NUM	8	Scan, by 3 Surrogates (Primary Ion)	LabData
IA.C12	ICSSR	(6,3)	NUM	8	Retention Time, by 3 Surrogates (Primary Ion)	LabData

4.0 Continuing Calibration Master File and Ancillary File

In the Continuing Calibration Master File, a record contains all quantitation report and computed data for each performance check 1/continuing calibration analysis and performance check 2 analysis run for an analytic shift on the GC/MS. This data represents the second logical level in the data structure. Each continuing calibration record will have one or more field sample or QC sample records pointing to it.

4.1 Logical Record Description

A logical record in this file contains data for a performance check1/continuing calibration analysis and performance check 2 for an analytic shift. The data elements are organized in groups, as follows:

- KEYS AND STATUS - the primary, unique identifier of each record in the file, along with any other (perhaps non-unique) keys, and the status flag.

- CHRONOLOGY - dates and times of significant events during the processing of the sample.

- DATA TRANSFER TRACKING - system dates used for maintenance of the data base.

- ANALYSIS LAB SAMPLE LOGIN DATA - data entered by the analytic laboratory when the sample was logged into their facility.

- ANALYSIS LAB SAMPLE EXTRACTION DATA - data generated by the analytic laboratory during the sample extraction process. This process removes the organic compounds from the solid soil material, resulting in a liquid suitable for analysis on the GC/MS.

- ANALYSIS LAB INJECTION DATA - data entered by the lab relating to injection of the sample in the GC/MS.

- ANALYSIS LAB INTERPRETATION DATA - data identifying the shift results file that the sample belonged to, the quantitation method used for each analyte, and the ion used for quantitation for each analyte. This data also contains the results of the GC/MS analysis when the peak height method of quantitation was used.

- CORRECTION FLAGS - flags used to indicate whether or not a particular element has been corrected/updated. If

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a flag is set "on" ("Y"), then the updated data is contained in this file, and the original data value is stored in the associated ancillary file record.

- ANALYSIS RAW DATA FOR CC/PC1 (after corrections, if any) AND PC2 - raw data generated by the GC/MS. This is essentially the same data contained on the quantitation report created by the GC/MS.

- LABDATA COMPUTATIONS FOR CONTINUING CALIBRATION - results calculated by the LabData system using the raw data generated by the GC/MS. It includes the continuing calibration response factor results, the QC criteria, and flags indicating whether or not the criteria were met.

- LABDATA PERFORMANCE CHECK DATA - the performance check ion ratios and the sensitivity results, the QC criteria for each, and flags indicating whether or not the criteria were met.

- DATA VALIDATION FLAGS AND COMMENTS - results of the data validation for the sample performed by EMSL-LV. It includes data validation checklist responses, comments, validation flags, and EMSL-LV usability flags.

- INTEGRATED DATA BASE AUDIT SYSTEM FLAGS - results of the automated audits and validations performed during the data base building process.

The ancillary file consists of three groups: KEYS, CHRONOLOGY, and DATA REPLACED BY CORRECTIONS. The last group corresponds to the ANALYSIS RAW DATA group in terms of data elements, but contains original data that has been replaced in the master file by corrected data.

4.2 Logical Subsets of the File - Special Screening

This file does not contain any data elements that define logical subsetting of the records.

4.3 Data Element Dictionaries

The data element dictionaries for the Continuing Calibration Master File and the Continuing Calibration Ancillary File follow this page.

LOVE CANAL HABITABILITY STUDY

CONTINUING CALIBRATION MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
******* Keys and Status **********						
CC.A01	CCANALID		CHAR	23	Continuing Calibration/Performance Check 1 Id (Lab Id + Lab Analysis Id of CC/PC1)	LabData
CC.A02	CCPC2ID		CHAR	23	Performance Check 2 Id (Lab Id + Lab Analysis Id of PC2)	LabData
CC.A03	CCSTATUS		CHAR	1	Status Flag Values: E = Validation Audit Failure blank = Passed Validation Audit	LabData
******* Chronology **********						
CC.B01	CCAADTE		NUM	8	CC/PC1 Analysis Lab Analysis Date	LabData
CC.B02	CCAATME		NUM	8	CC/PC1 Analysis Lab Analysis Time	LabData
CC.B03	PC2AADTE		NUM	8	PC2 Analysis Lab Analysis Date	LabData
CC.B04	PC2AATME		NUM	8	PC2 Analysis Lab Analysis Time	LabData
******* Data Transfer Tracking **********						
CC.C01	CCGENDTE		NUM	8	LabData Gen Date	LabData
CC.C02	CCGENTME		NUM	8	LabData Gen Time	LabData
CC.C03	CCADDDTE		NUM	8	DB Add Date	IntDBBld
CC.C04	CCADDTME		NUM	8	DB Add Time	IntDBBld
CC.C05	CCUPDDTE		NUM	8	DB Most Recent Update Date	IntDBBld
CC.C06	CCUPDTME		NUM	8	DB Most Recent Update Time	IntDBBld
CC.C07	CCUPDCNT		NUM	8	DB Update Count	IntDBBld
******* Analysis Lab Sample Login Data **********						
CC.D01	CCSMPL	(2)	CHAR	10	Sample Id for CC/PC1 and PC2	LabData
CC.D02	CCALID		CHAR	3	Analysis Lab Id Values: AQI CAA CEC EMS MGM NU2 = Contingency samples - for possible replacement; prepped and stored but never analyzed NUS VER blanks = no analysis performed; therefore no Lab Id	LabData
******* Analysis Lab Injection Data (For CC/PC1 and PC2) **********						
CC.E01	CCINSTID		CHAR	15	GC/MS Instrument Id	LabData
CC.E02	CCANLST	(2)	CHAR	8	GC/MS Analyst, by 2 Analyses	LabData

LOVE CANAL HABITABILITY STUDY

CONTINUING CALIBRATION MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
CC.E03	CCFILE	(2)	CHAR	15	GC/MS Datafile Id, by 2 Analyses	LabData
CC.E04	CCINJVL	(2)	NUM	8	Injection Volume (ul), by 2 Analyses	LabData
******* Analysis Lab Interpretation Data **********						
CC.F01	CCQFILE		CHAR	12	GC/MS Shift Results File Name For CC/PC1 ONLY:	LabData
CC.F02	CCQMTH	(8,3)	CHAR	1	Quantitation Method Flag, by 8 LCICs, by 3 Ions Values: blank) or) = GC/MS Automatic Area Quantitation A) H = Peak Height Quantitation M = GC/MS Manual Quantitation O = Computed using area by LabData with correction data	LabData
CC.F03	CCQION	(8)	CHAR	1	LCIC Quantitation Ion Selection, By 8 LCICs Values: blank = Primary ion area used for quantitation S = Secondary ion area used for quantitation T = Tertiary ion area used for quantitation	LabData
CC.F04	CCLCPH	(8,3)	NUM	8	Peak Height, by 8 LCICs, by 3 Ions	LabData
CC.F05	CCISPH	(5)	NUM	8	Peak Height, by 5 Int. Stds. (Primary Ion)	LabData
CC.F06	CCPYRPH		NUM	8	Peak Height Pyrene-D10 (Secondary Ion)	LabData
CC.F07	CCSSPH	(3)	NUM	8	Peak Height, by 3 Surrogates (Primary Ion)	LabData
CC.F08	CCHLCS	(8,3)	NUM	8	Scan for Peak Height, by 8 LCICs, by 3 Ions	LabData
CC.F09	CCHLCR	(8,3)	NUM	8	Retention Time for Peak Height, by 8 LCICs, by 3 Ions	LabData
CC.F10	CCHISS	(5)	NUM	8	Scan for Peak Height, by 5 Int. Stds.,	LabData
CC.F11	CCHISR	(5)	NUM	8	Retention Time for Peak Height, by 5 Int. Stds.	LabData
CC.F12	CCHPYRS		NUM	8	Scan for Peak Height for Pyrene-D10	LabData
CC.F13	CCHPYRR		NUM	8	Retention Time for Peak Height for Pyrene-D10	LabData
CC.F14	CCHSSS	(3)	NUM	8	Scan for Peak Height, by 3 Surrogates Values: 0 = Peak height scan not performed nnnn = Scan number for peak height scan performed	LabData
CC.F15	CCHSSR	(3)	NUM	8	Retention Time for Peak Height, by 3 Surrogates	LabData
******* Correction Flags (For CC/PC1 ONLY) **********						
					Values: Y = data corrected, original data stored in ancillary file blank = data not corrected, no data stored in ancillary file	
CC.G01	CCCDATE		CHAR	1	Analysis Lab Analysis Date	LabData

LOVE CANAL HABITABILITY STUDY

CONTINUING CALIBRATION MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
CC.G02	CCCTIME		CHAR	1	Analysis Lab Analysis Time	LabData
CC.G03	CCCANAL		CHAR	1	Analyst	LabData
CC.G04	CCCLCA	(8,3)	CHAR	1	Area, by 8 LCICs, by 3 Ions	LabData
CC.G05	CCCLCS	(8,3)	CHAR	1	Scan, by 8 LCICs, by 3 Ions	LabData
CC.G06	CCCLCR	(8,3)	CHAR	1	Retention Time, by 8 LCICs, by 3 Ions	LabData
CC.G07	CCCISA	(5)	CHAR	1	Area, by 5 Int. Stds. (Primary Ion)	LabData
CC.G08	CCCISS	(5)	CHAR	1	Scan, by 5 Int. Stds. (Primary Ion)	LabData
CC.G09	CCCISR	(5)	CHAR	1	Retention Time, by 5 Int. Stds. (Primary Ion)	LabData
CC.G10	CCCPYRA		CHAR	1	Area Pyrene-D10 (Secondary Ion)	LabData
CC.G11	CCCPYRS		CHAR	1	Scan Pyrene-D10 (Secondary Ion)	LabData
CC.G12	CCCPYRR		CHAR	1	Retention Time Pyrene-D10 (Secondary Ion)	LabData
CC.G13	CCCSSA	(3)	CHAR	1	Area, by 3 Surrogates (Primary Ion)	LabData
CC.G14	CCCSSS	(3)	CHAR	1	Scan, by 3 Surrogates (Primary Ion)	LabData
CC.G15	CCCSSR	(3)	CHAR	1	Retention Time, by 3 Surrogates (Primary Ion)	LabData
******* Analysis Raw Data For CC/PC1 (After Corrections, if any) and PC2 **********						
CC.H01	CCLCA	(2,8,3)	NUM	8	Area, by 2 Analyses, by 8 LCICs, by 3 Ions	LabData
CC.H02	CCLCS	(2,8,3)	NUM	8	Scan, by 2 Analyses, by 8 LCICs, by 3 Ions	LabData
CC.H03	CCLCR	(2,8,3)	NUM	8	Retention Time, by 2 Analyses, by 8 LCICs, by 3 Ions	LabData
CC.H04	CCISA	(2,5)	NUM	8	Area, by 2 Analyses, by 5 Int. Stds. (Primary Ion)	LabData
CC.H05	CCPYRA	(2)	NUM	8	Area Pyrene-D10 (Secondary Ion), by 2 Analyses	LabData
CC.H06	CCISS	(2,5)	NUM	8	Scan, by 2 Analyses, by 5 Int. Stds. (Primary Ion)	LabData
CC.H07	CCPYRS	(2)	NUM	8	Scan Pyrene-D10 (Secondary Ion), by 2 Analyses	LabData
CC.H08	CCISR	(2,5)	NUM	8	Retention Time, by 2 Analyses, by 5 Int. Stds. (Primary Ion)	LabData
CC.H09	CCPYRR	(2)	NUM	8	Retention Time Pyrene-D10 (Secondary Ion), by 2 Analyses	LabData
CC.H10	CCSSA	(2,3)	NUM	8	Area, by 2 Analyses, by 3 Surrogates (Primary Ion)	LabData
CC.H11	CCSSS	(2,3)	NUM	8	Scan, by 2 Analyses, by 3 Surrogates (Primary Ion)	LabData
CC.H12	CCSSR	(2,3)	NUM	8	Retention Time, by 2 Analyses, by 3 Surrogates (Primary Ion)	LabData
******* LabData Computations for Continuing Calibration **********						
CC.I01	CCRFA	(11,3)	NUM	8	Response Factors using Area, by 8 LCICs and 3 Surrogates, by 3 Ions	*LabData
CC.I02	CCRFPH	(11,3)	NUM	8	Response Factors using Peak Height, by 8 LCICs and 3 Surrogates, by 3 Ions	*LabData

LOVE CANAL HABITABILITY STUDY

CONTINUING CALIBRATION MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
CC.I03	CCRIR	(11)	NUM	8	Target Ion Ratios for Id Criteria using Theoretical Values, by 8 LCICs and 3 Surrogates	LabData
CC.I04	CCPDRF	(11)	NUM	8	% Dev. From Mean of Response Factors, by 8 LCICs and 3 Surrogates	LabData
CC.I05	CCPDC	(11)	NUM	8	% Dev. Criteria, by 8 LCICs and 3 Surrogates	LabData
CC.I06	CCPDF	(11)	CHAR	1	Flag for % Dev out of criteria, by 8 LCICs and 3 Surrogates Values: * = % deviation out of criteria; greater than 40% + = % deviation out of criteria; 20% < % dev <= 40% blank = % deviation within criteria	LabData
CC.I07	CCPDOUT		NUM	8	Number of % Dev Out of Criteria	LabData
CC.I08	CCRR	(8,3)	NUM	8	Relative Retention Time, by 8 LCICs, by 3 Ions	*LabData
******* LabData Performance Check Data **********						
CC.J01	PCIR	(2,9)	NUM	8	Ion Ratios, by 2 analyses (PC1, PC2), by 8 LCICs and Pyrene-D10	*LabData
CC.J02	PCIRLC	(2,9)	NUM	8	Ion Criteria lower value, by 2 analyses (PC1, PC2), by 8 LCICs and Pyrene-D10	LabData
CC.J03	PCIRUC	(2,9)	NUM	8	Ion Criteria upper value, by 2 analyses (PC1, PC2), by 8 LCICs and Pyrene-D10	LabData
CC.J04	PCIRF	(2,9)	CHAR	1	Flag for Ion ratio Out of Criteria, by 2 analyses (PC1, PC2), by 8 LCICs and Pyrene-D10 Values: * = out of criteria blank = within criteria	*LabData
CC.J05	PCIROUT	(2)	NUM	8	Number of PC Vals Out of Criteria, by 2 analyses (PC1, PC2)	LabData
CC.J06	PCBLSEP		CHAR	1	Baseline Separation Values: blank = no baseline separation Y = baseline separation between CNP isomers	LabData
CC.J07	PCPV	(3)	NUM	8	% valley (PC1/CNP, PC2/CNP, PC2/BHC)	LabData
CC.J08	PCPVF	(3)	CHAR	1	Flag for % valley (PC1/CNP, PC2/CNP, PC2/BHC) Out of Criteria Values: * = % valley out of criteria; greater than 40% + = % valley out of criteria; 20% < % dev <= 40% blank = % valley within criteria	*LabData
CC.J09	PCPVC	(3)	NUM	8	% Valley Criteria (PC1/CNP, PC2/CNP, PC2/BHC)	LabData
CC.J10	PCSNR	(2,2)	NUM	8	Signal to Noise Ratio(PC1/BHC,PC2/BHC,PC1/TeBB,PC2/TeBB)	LabData

LOVE CANAL HABITABILITY STUDY

CONTINUING CALIBRATION MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
CC.J11	PCSNRF	(2,2)	CHAR	1	Signal to Noise Ratio Out of Crit. Flag (PC1/BHC,PC2/BHC,PC1/TeBB,PC2/TeBB) Values: * = out of criteria blank = within criteria	*LabData
CC.J12	PCSNRC	(2,2)	NUM	8	Signal to Noise Ratio(PC1/BHC,PC2/BHC,PC1/TeBB,PC2/TeBB) Criteria	LabData
******* Data Validation Flags **********						
	Values: (currently not available)					
CC.K01	DVDELIV		CHAR	1	Are all deliverables present	DataVal
CC.K02	DVMISS	(7)	CHAR	40	Missing deliverables	DataVal
CC.K03	DVRES	(7)	CHAR	8	Dates resolved	DataVal
CC.K04	DVPC1A		CHAR	1	PC1 Compare percent valley SICPS	DataVal
CC.K05	DVPC1B		CHAR	1	PC1 Compare signal to noise ratios with raw data	DataVal
CC.K06	DVPC1C		CHAR	1	PC1 Check ion ratio criteria	DataVal
CC.K07	DVPC1D		CHAR	2	PC1 Check chromatography	DataVal
CC.K08	DVPC1E		CHAR	2	PC1 Check quantitation reports for evidence of editing	DataVal
CC.K09	DVPC1F		CHAR	2	PC1 Miscellaneous	DataVal
CC.K10	DVPC1DT		CHAR	8	PC1 Date	DataVal
CC.K11	DVPC1TM		CHAR	8	PC1 Time	DataVal
CC.K12	DVPCMDP		CHAR	1	Is this a PC2 midpoint for 16 hour analytical run?	DataVal
CC.K13	DVHALF		CHAR	12	First half shift result file name if exists	DataVal
CC.K14	DVPC1CM	(3)	CHAR	60	PC1 Comments	DataVal
CC.K15	DVPC2A		CHAR	1	PC2 Compare percent valley SICPS	DataVal
CC.K16	DVPC2B		CHAR	1	PC2 Compare signal to noise ratios with raw data	DataVal
CC.K17	DVPC2C		CHAR	1	PC2 Check ion ratio criteria	DataVal
CC.K18	DVPC2D		CHAR	2	PC2 Check chromatography	DataVal
CC.K19	DVPC2E		CHAR	2	PC2 Check quantitation reports for evidence of editing	DataVal
CC.K20	DVPC2F		CHAR	2	PC2 Miscellaneous	DataVal
CC.K21	DVPC2DT		CHAR	8	PC2 Date	DataVal
CC.K22	DVPC2TM		CHAR	8	PC2 Time	DataVal
CC.K23	DVPC2CM	(3)	CHAR	60	PC2 Comments	DataVal
CC.K24	DVEPAA		CHAR	2	EPA Chk. Std. Recoveries within acceptance windows	DataVal
CC.K25	DVEPAB		CHAR	2	EPA Chk. Std. Check chromatography	DataVal
CC.K26	DVEPAC		CHAR	2	EPA Chk. Std. Check quantitation reports	DataVal
CC.K27	DVEPAD		CHAR	2	EPA Chk. Std. Miscellaneous	DataVal
CC.K28	DVEPASMP		CHAR	10	EPA Chk. Std. Sample Id	DataVal
CC.K29	DVEPACM	(3)	CHAR	60	EPA Comments	DataVal
CC.K30	DVCCCALA		CHAR	1	Continuing Calibration Internal standard areas	DataVal
CC.K31	DVCCCALB		CHAR	1	Continuing Calibration Check retention time differences	DataVal
CC.K32	DVCCCALC		CHAR	2	Continuing Calibration Miscellaneous	DataVal
CC.K33	DVCCDT		CHAR	8	Continuing Calibration Date	DataVal
CC.K34	DVCCTM		CHAR	8	Continuing Calibration Time	DataVal
CC.K35	DVCCCOM	(3)	CHAR	60	Continuing Calibration Comments	DataVal

LOVE CANAL HABITABILITY STUDY

CONTINUING CALIBRATION MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
******* Integrated DB Audit System Flags **********						
CC.L01	CCRECALC		CHAR	1	Flag for calculation discrepancies Values: * = Discrepancy blank = No discrepancy	IntDBBld

LOVE CANAL HABITABILITY STUDY

CONTINUING CALIBRATION ANCILLARY FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
******* Keys **********						
CA.A01	CCANALID		CHAR	23	Continuing Calibration/Performance Check 1 Id (Lab Id + Lab Analysis Id of CC/PC1)	LabData
******* Data Transfer Tracking **********						
CA.B01	CCGENDTE		NUM	8	LabData Gen Date	LabData
CA.B02	CCGENTME		NUM	8	LabData Gen Time	LabData
CA.B03	CCADDDTE		NUM	8	DB Add Date	IntDBBld
CA.B04	CCADDTME		NUM	8	DB Add Time	IntDBBld
CA.B05	CCUPDDTE		NUM	8	DB Most Recent Update Date	IntDBBld
CA.B06	CCUPDTME		NUM	8	DB Most Recent Update Time	IntDBBld
CA.B07	CCUPDCNT		NUM	8	DB Update Count	IntDBBld
******* Data Replaced by Corrections **********						
CA.C01	CCLCA	(2,8,3)	NUM	8	Area, by 2 Analyses, by 8 LCICs, by 3 Ions	LabData
CA.C02	CCLCS	(2,8,3)	NUM	8	Scan, by 2 Analyses, by 8 LCICs, by 3 Ions	LabData
CA.C03	CCLCR	(2,8,3)	NUM	8	Retention Time, by 2 Analyses, by 8 LCICs, by 3 Ions	LabData
CA.C04	CCISA	(2,5)	NUM	8	Area, by 2 Analyses, by 5 Int. Stds. (Primary Ion)	LabData
CA.C05	CCPYRA	(2)	NUM	8	Area Pyrene-D10 (Secondary Ion), by 2 Analyses	LabData
CA.C06	CCISS	(2,5)	NUM	8	Scan, by 2 Analyses, by 5 Int. Stds. (Primary Ion)	LabData
CA.C07	CCPYRS	(2)	NUM	8	Scan Pyrene-D10 (Secondary Ion), by 2 Analyses	LabData
CA.C08	CCISR	(2,5)	NUM	8	Retention Time, by 2 Analyses, by 5 Int. Stds. (Primary Ion)	LabData
CA.C09	CCPYRR	(2)	NUM	8	Retention Time Pyrene-D10 (Secondary Ion), by 2 Analyses	LabData
CA.C10	CCSSA	(2,3)	NUM	8	Area, by 2 Analyses, by 3 Surrogates (Primary Ion)	LabData
CA.C11	CCSSS	(2,3)	NUM	8	Scan, by 2 Analyses, by 3 Surrogates (Primary Ion)	LabData
CA.C12	CCSSR	(2,3)	NUM	8	Retention Time, by 2 Analyses, by 3 Surrogates (Primary Ion)	LabData

5.0 Quality Control (QC) Sample Master File and Ancillary File

In the QC Sample Master File, a record contains all quantitation report and computed data for QC samples. Each analytic run, or "shift," containing field samples was required to have certain QC samples run as well. Depending upon various factors, one or more different types of QC samples would be run in each shift.

A pointer, or key, is present to link to each sample's continuing calibration record.

5.1 Logical Record Description

A logical record contains the data for one QC sample. The data elements are organized in groups, as follows:

- KEYS AND STATUS - the primary, unique identifier of each record in the file, along with any other (perhaps non-unique) keys, and the status flag.

- CHRONOLOGY - dates and times of significant events during the processing of the sample.

- DATA TRANSFER TRACKING - system dates used for maintenance of the data base.

- FIELD SAMPLING DATA - data generated during the collection of the sample in the field.

- PREPARATION LAB DATA - data generated during the preparation of the sample. The preparation process consisted of removing the soil from the sampling tube, homogenizing the soil, placing the soil in a container for shipment, and shipping it to an analytical laboratory.

- ANALYSIS LAB SAMPLE LOGIN DATA - data entered by the analytic laboratory when the sample was logged into their facility.

- ANALYSIS LAB SAMPLE EXTRACTION DATA - data generated by the analytic laboratory during the sample extraction process. This process removes the organic compounds from the solid soil material, resulting in a liquid suitable for analysis on the GC/MS.

- ANALYSIS LAB INJECTION DATA - data entered by the lab relating to injection of the sample in the GC/MS.

- ANALYSIS LAB INTERPRETATION DATA - data identifying the shift results file that the sample belonged to,

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the quantitation method used for each analyte, and the ion used for quantitation for each analyte. This data also contains the results of the GC/MS analysis when the peak height method of quantitation was used.

- CORRECTION FLAGS - flags used to indicate whether or not a particular element has been corrected/updated. If a flag is set "on" ("Y"), then the updated data is contained in this file, and the original data value is stored in the associated ancillary file record.

- ANALYSIS RAW DATA - (after corrections, if any) raw data generated by the GC/MS. This is essentially the same data contained on the quantitation report created by the GC/MS.

- LABDATA COMPUTATIONS FOR QC SAMPLES - results calculated by the LabData system using the raw data generated by the GC/MS and additional data entered by the laboratory. It includes the concentration results after the identification criteria (ID) have been applied, pre-criteria concentrations, ID criteria results, and flags indicating whether or not the criteria were met.

- LABDATA COMPUTATIONS FOR SURROGATE STANDARDS - results computed by LabData for the surrogate recoveries for the sample analysis. Included are the percent recoveries, flags indicating whether or not the recovery met the criteria, and the criteria.

- LABDATA COMPUTATIONS FOR INTERNAL STANDARDS - results computed by LabData for the internal standards for the sample analysis. Included are retention time and area criteria check results.

- LABDATA COMPUTATIONS FOR METHOD HOLDING BLANK - concentrations for secondary and tertiary ions, QC criteria results, and flags indicating whether or not the criteria were met.

- LABDATA MATRIX SPIKE DATA - quantity of the spike, percent recovery, QC criteria results, and flags indicating whether or not the criteria were met.

- DATA VALIDATION FLAGS AND COMMENTS - results of the data validation for the sample performed by EMSL-LV. It includes data validation checklist responses, comments, validation flags, and EMSL-LV usability flags.

- INTEGRATED DATA BASE AUDIT SYSTEM FLAGS - results of the automated audits and validations performed during the data base building process.

The ancillary file consists of three groups: KEYS, CHRONOLOGY, and DATA REPLACED BY CORRECTIONS. The last group corresponds to the ANALYSIS RAW DATA group in terms of data elements, but contains original data that has been replaced in the master file by corrected data.

5.2 Logical Subsets of the File - Special Screening

The primary grouping of logical subsets in the QC Sample Master File is based upon sample types. The table below depicts these sample types, and sub-groups within each sample type.

Sample Type Code (QCTYPE)	Description
QCEMSL	EMSL Blind QC samples - samples spiked with known concentrations of LCICs, but the levels were not known by the analytic laboratory. A Blind QC sample was extracted with each extraction batch of samples and analyzed. If a given level of recovery was not achieved in the Blind QC, then the laboratory had to re-extract all the field samples in the extraction batch.
MS	The Matrix Spike and Matrix Spike Duplicate samples MSD were created by splitting every twentieth field sample into three parts. One third was treated as a normal field sample (i.e., the "native" sample in a native/MS/MSD set of analyses), one-third as an MS analysis, and one-third as the MSD. Each MS and MSD was then spiked with a fixed amount of LCICs. The results were then used for QC purposes. See Section 8.5 for a description of how to merge the native samples with MS/MSD analyses.
BLM	The Method Blank was a blank sample, prepared by the analytic laboratory, containing no known levels of LCICs. This sample was then extracted in a batch of field samples, subjected to the same handling and storage, and analyzed with the field samples. The results were not to indicate any significant levels of LCICs. If significant levels of LCICs were found, the laboratory had to re-extract all field samples in that extraction batch.

BLR — The Reagent Blank was also a blank sample, made up from the solvents used during the sample extraction process and analyzed to determine if the analysis process was introducing LCIC contamination into the field samples.

As was the case with the Field Samples in FSFILE, the data usability flags associated with the sample results must be merged in from the FORM I file. Section 8 contains directions for combining files.

5.3 Data Element Dictionaries

The data element dictionaries for the Quality Control Sample Master File and the Quality Control Sample Ancillary File follow this page.

LOVE CANAL HABITABILITY STUDY

QUALITY CONTROL MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
******* Keys and Status **********						
QC.A01	QCANALID		CHAR	23	QC Lab Analysis Id - (Lab Id + Lab Analysis Id)	LabData
QC.A02	QCSTATUS		CHAR	1	Status Flag Values: E = Validation Audit Failure blank = Passed Validation Audit	IntDBBld
QC.A03	CLEANHS		CHAR	8	Original Project Id (HS Number)	IntDBBld
******* Chronology **********						
QC.B01	QCALDTE		NUM	8	Analysis Lab Login Date	LabData
QC.B02	QCAEDTE		NUM	8	Analysis Lab Extract Date	LabData
QC.B03	QCAADTE		NUM	8	Analysis Lab Analysis Date	LabData
QC.B04	QCAATME		NUM	8	Analysis Lab Analysis Time	LabData
QC.B05	QCDBDTE		NUM	8	Data Validation Date	DataVal
******* Data Transfer Tracking **********						
QC.C01	QCGENDTE		NUM	8	LabData Gen Date	LabData
QC.C02	QCGENTME		NUM	8	LabData Gen Time	LabData
QC.C03	QCADDDTE		NUM	8	DB Add Date	IntDBBld
QC.C04	QCADDTME		NUM	8	DB Add Time	IntDBBld
QC.C05	QCUPDDTE		NUM	8	DB Most Recent Update Date	IntDBBld
QC.C06	QCUPDTME		NUM	8	DB Most Recent Update Time	IntDBBld
QC.C07	QCUPDCNT		NUM	8	DB Update Count	IntDBBld
******* Analysis Lab Sample Login Data **********						
QC.D01	QCSMPL		CHAR	8	QC Sample Id from LabData (the Project Sample Id)	LabData
QC.D02	QCALID		CHAR	3	Analytic Laboratory Id Values: AQI CAA CEC EMS MGM NU2 = Contingency samples - for possible replacement; prepped and stored but never analyzed NUS VER blanks = no analysis performed; therefore no Lab Id	LabData
QC.D03	QCRERUN		CHAR	2	Re-run Flag	currently not used
QC.D04	QCRRSTAT		CHAR	1	Re-run Type	currently not used
QC.D05	QCORIG		CHAR	1	Orig. Found Flag	currently not used

LOVE CANAL HABITABILITY STUDY
QUALITY CONTROL MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
QC.D06	QCTYPE		CHAR	6	QC Sample Type Values: MS = Matrix Spike MSD = Matrix Spike Duplicate BLM = Method Blank BLR = Reagent Blank QCEMSL = EMSL Blind QC Sample	LabData
******* Analysis Lab Sample Extraction Data **********						
QC.E01	QCTWTEXT		NUM	8	Target Weight to Extract (gm)	LabData
QC.E02	QCWTEXT		NUM	8	Weight Extracted (gm)	LabData
QC.E03	QCMOIST		NUM	8	Percent Moisture	LabData
QC.E04	QCCONCDF		NUM	8	Concentration Dilution Factor	LabData
******* Analysis Lab Injection Data **********						
QC.F01	QCINSTID		CHAR	15	GC/MS Instrument Id	LabData
QC.F02	QCANLST		CHAR	8	GC/MS Analyst	LabData
QC.F03	QCFILE		CHAR	15	GC/MS Datafile Id	LabData
QC.F04	QCINJVOL		NUM	8	Injection Volume (ul)	LabData
******* Analysis Lab Interpretation Data **********						
QC.G01	QCQFILE		CHAR	12	GC/MS Shift Results File Name	LabData
QC.G02	QCQMTH	(8,3)	CHAR	1	Quantitation Method Flag, by 8 LCICs, by 3 Ions Values: blank) or) = GC/MS Automatic Area Quantitation A) H = Peak Height Quantitation M = GC/MS Manual Quantitation O = Computed using area by LabData with correction data	LabData
QC.G03	QCQION	(8)	CHAR	1	LCIC Quantitation Ion Selection, by 8 LCICs Values: blank = Primary ion used for quantitation S = Secondary ion used for quantitation T = Tertiary ion used for quantiation	LabData
QC.G04	QCLCPH	(8,3)	NUM	8	Peak Height, by 8 LCICs, by 3 Ions	LabData
QC.G05	QCISPH	(5)	NUM	8	Peak Height, by 5 Int. Stds. (Primary Ion)	LabData
QC.G06	QCPYRPH		NUM	8	Peak Height Pyrene-D10 (Secondary Ion)	LabData
QC.G07	QCSSPH	(3)	NUM	8	Peak Height, by 3 Surrogates (Primary Ion)	LabData
QC.G08	QCHLCS	(8,3)	NUM	8	Scan for Peak Height, by 8 LCICs, by 3 Ions	LabData
QC.G09	QCHLCR	(8,3)	NUM	8	Retention Time for Peak Height, by 8 LCICs, by 3 Ions	LabData
QC.G10	QCHISS	(5)	NUM	8	Scan for Peak Height, by 5 Int. Stds.	LabData
QC.G11	QCHISR	(5)	NUM	8	Retention Time for Peak Height, by 5 Int. Stds.	LabData
QC.G12	QCHPYRS		NUM	8	Scan for Peak Height for Pyrene-D10	LabData

LOVE CANAL HABITABILITY STUDY

QUALITY CONTROL MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
QC.G13	QCHPYRR		NUM	8	Retention Time for Peak Height for Pyrene-D10	LabData
QC.G14	QCHSSS	(3)	NUM	8	Scan for Peak Height, by 3 Surrogates	LabData
QC.G15	QCHSSR	(3)	NUM	8	Retention Time for Peak Height, by 3 Surrogates	LabData
******* Correction Flags **********						
		Values:				
		blank = data has not been corrected				
		"Y" = data has been corrected; original data in ancillary file				
QC.H01	QCCDATE		CHAR	1	Analysis Lab Analysis Date	LabData
QC.H02	QCCTIME		CHAR	1	Analysis Lab Analysis Time	LabData
QC.H03	QCCANAL		CHAR	1	Analyst	LabData
QC.H04	QCCLCA	(8,3)	CHAR	1	Area, by 8 LCICs, by 3 Ions	LabData
QC.H05	QCCLCS	(8,3)	CHAR	1	Scan, by 8 LCICs, by 3 Ions	LabData
QC.H06	QCCLCR	(8,3)	CHAR	1	Retention Time, by 8 LCICs, by 3 Ions	LabData
QC.H07	QCCISA	(5)	CHAR	1	Area, by 5 Int. Stds. (Primary Ion)	LabData
QC.H08	QCCISS	(5)	CHAR	1	Scan, by 5 Int. Stds. (Primary Ion)	LabData
QC.H09	QCCISR	(5)	CHAR	1	Retention Time, by 5 Int. Stds. (Primary Ion)	LabData
QC.H10	QCCPYRA		CHAR	1	Area Pyrene-D10 (Secondary Ion)	LabData
QC.H11	QCCPYRS		CHAR	1	Scan Pyrene-D10 (Secondary Ion)	LabData
QC.H12	QCCPYRR		CHAR	1	Retention Time Pyrene-D10 (Secondary Ion)	LabData
QC.H13	QCCSSA	(3)	CHAR	1	Area, by 3 Surrogates (Primary Ion)	LabData
QC.H14	QCCSSS	(3)	CHAR	1	Scan, by 3 Surrogates (Primary Ion)	LabData
QC.H15	QCCSSR	(3)	CHAR	1	Retention Time, by 3 Surrogates (Primary Ion)	LabData
******* Analysis Raw Data (After Corrections, if any) **********						
QC.I01	QCLCA	(8,3)	NUM	8	Area, by 8 LCICs, by 3 Ions	LabData
QC.I02	QCLCS	(8,3)	NUM	8	Scan, by 8 LCICs, by 3 Ions	LabData
QC.I03	QCLCR	(8,3)	NUM	8	Retention Time, by 8 LCICs, by 3 Ions	LabData
QC.I04	QCISA	(5)	NUM	8	Area, by 5 Int. Stds. (Primary Ion)	LabData
QC.I05	QCPYRA		NUM	8	Area Pyrene-D10 (Secondary Ion)	LabData
QC.I06	QCISS	(5)	NUM	8	Scan, by 5 Int. Stds. (Primary Ion)	LabData
QC.I07	QCPYRS		NUM	8	Scan Pyrene-D10 (Secondary Ion)	LabData
QC.I08	QCISR	(5)	NUM	8	Retention Time, by 5 Int. Stds. (Primary Ion)	LabData
QC.I09	QCPYRR		NUM	8	Retention Time Pyrene-D10 (Secondary Ion)	LabData
QC.I10	QCSSA	(3)	NUM	8	Area, by 3 Surrogates (Primary Ion)	LabData
QC.I11	QCSSS	(3)	NUM	8	Scan, by 3 Surrogates (Primary Ion)	LabData
QC.I12	QCSSR	(3)	NUM	8	Retention Time, by 3 Surrogates (Primary Ion)	LabData
******* LabData Computations for QC Samples **********						
QC.J01	QCRR	(8)	NUM	8	Relative Retention Time, by 8 LCICs (Quantitation Ion)	*LabData
QC.J02	QCRRC	(8)	NUM	8	Relative Retention Time Criteria, by 8 LCICs	LabData

LOVE CANAL HABITABILITY STUDY
QUALITY CONTROL MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
QC.J03	QCRRF	(8)	CHAR	1	Flag for Rel. Ret. Time Out of Criteria, by 8 LCICs Values: * = Out of criteria blank = Within criteria	*LabData
QC.J04	QCCONCB	(8)	NUM	8	PreID-criteria Concentration, by 8 LCICs (i.e.,primary ion equivalent concentration)	*LabData
QC.J05	QCCONCA	(8)	NUM	8	Id Criteria applied Concentration, by 8 LCICs	*LabData
QC.J06	QCIRAT	(8)	NUM	8	Ion Ratio, by 8 LCICs	*LabData
QC.J07	QCIONF	(8)	CHAR	1	Flag for All Ions Being Present, by 8 LCICs Values: * = All ions present blank = One or more ions not present	*LabData
QC.J08	QCMINS	(8)	NUM	8	Minimum Scan Number of 3 Ions, by 8 LCICs	LabData
QC.J09	QCMAXS	(8)	NUM	8	Maximum Scan Number of 3 Ions, by 8 LCICs	LabData
QC.J10	QCRANG	(8)	NUM	8	Scan Range (Max - Min), by 8 LCICs	*LabData
QC.J11	QCRANGF	(8)	CHAR	1	Flag for Scan range >2, by 8 LCICs Values: * = scan range greater than 2 blank = scan range less than or equal to 2	*LabData
QC.J12	QCIDEVT	(8)	NUM	8	Ion Ratio % Dev. from Theoretical Values, by 8 LCICs	*LabData
QC.J13	QCIDEVF	(8)	CHAR	1	Flag for Ion ratio % Dev. Out of Criteria, by 8 LCICs Values: * = % dev. out of criteria; greater than 40% + = % dev. out of criteria; 20% < % dev <= 40% blank = % dev. within criteria	*LabData
QC.J14	QCPRESCR		CHAR	3	Flag for Analysis Pre-screen Values: 'MS ' = GC/MS pre-screening performed 'ECD' = GC/ECD pre-screening performed blanks = no pre-screening done	LabData
QC.J15	QCSULFUR		CHAR	1	Flag for Sulphur Cleanup Performed Values: Y = sulphur cleanup performed blank or N = no sulphur cleanup performed	LabData
******* LabData Computations for Surrogate Standards **********						
QC.K01	QCPR	(3)	NUM	8	% Recovery by 3 Surrogates	*LabData
QC.K02	QCPRF	(3)	CHAR	1	Flag for % Rec. Out of Criteria, by 3 Surrogates Values: * = Out of criteria blank = Within criteria	*LabData
QC.K03	QCSSADD	(3)	NUM	8	Amount of added(ng), by 3 Surrogates	LabData
QC.K04	QCPRCL	(3)	NUM	8	% Recovery Criteria lower limit, by 3 Surrogates	LabData
QC.K05	QCPRCU	(3)	NUM	8	% Recovery Criteria upper limit, by 3 Surrogates	LabData
QC.K06	QCPROUT		NUM	8	Number of % Rec. Out of Criteria	*LabData

LOVE CANAL HABITABILITY STUDY

QUALITY CONTROL MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
******* LabData Computations for Internal Standards **********						
QC.L01	QCISADD		NUM	8	Internal Standard Quantity Added (in nanograms)	LabData
QC.L02	QCRD	(5)	NUM	8	Ret. Time Difference From CC Val, by 5 Int Stds	*LabData
QC.L03	QCAD	(5)	NUM	8	Area Difference % From CC Val, by 5 Int Stds	*LabData
QC.L04	QCRF	(5)	CHAR	1	Flag for Ret. Time Out of Criteria, by 5 Int Stds Values: * = Out of criteria blank = Within criteria	*LabData
QC.L05	QCAF	(5)	CHAR	1	Flag for Area Out of Criteria, by 5 Int Stds Values: * = Out of criteria blank = Within criteria	*LabData
QC.L06	QCRDC	(5)	NUM	8	Retention Time Difference Criteria, by 5 Int Stds	LabData
QC.L07	QCADCL	(5)	NUM	8	Area % Diff. Crit. lower limit, by 5 Int Stds	LabData
QC.L08	QCADCU	(5)	NUM	8	Area % Diff. Crit. upper limit, by 5 Int Stds	LabData
******* LabData Computations for Method Holding Blank **********						
QC.M01	QCSICON	(8)	NUM	8	Concentration, by 8 LCICs (secondary ion)	*LabData
QC.M02	QCTICON	(8)	NUM	8	Concentration, by 8 LCICs (tertiary ion)	*LabData
QC.M03	QCMAXCON		NUM	8	Maximum Conc. Criteria	LabData
QC.M04	QCCONF	(8,3)	CHAR	1	Concentration Out of Criteria Flag, by 8 LCICs, by 3 Ions Values: * = Out of criteria blank = Within criteria	*LabData
******* LabData Matrix Spike Data **********						
QC.N01	QCSADDED		NUM	8	Amount of Spike Added (ng)	LabData
QC.N02	QCSRECV	(8)	NUM	8	Amount of Spike Recovered (ng), by 8 LCICs	*LabData
QC.N03	QCSPRCU	(8)	NUM	8	% Recovery Upper Limit Criteria, by 8 LCICs	LabData
QC.N04	QCSPRCL	(8)	NUM	8	% Recovery Lower Limit Criteria, by 8 LCICs	LabData
QC.N05	QCSPRL	(8)	NUM	8	% Recovery Relative % Dev. Limit, by 8 LCICs	LabData
QC.N06	QCSPR	(8)	NUM	8	% Recovery, by 8 LCICs	*LabData
QC.N07	QCSPDD	(8)	NUM	8	Relative % Dev. of MS/MSD % Recoveries, by 8 LCICs	*LabData
******* Data Validation Flags and Comments **********						
	Values: (currently not available)					
QC.O01	DVCHKA		CHAR	2	Recoveries within acceptance criteria	DataVal
QC.O02	DVCHKB		CHAR	2	Check chromatography	DataVal
QC.O03	DVCHKC		CHAR	2	Check quantitation reports	DataVal
QC.O04	DVCHKD		CHAR	2	Blind QC Samples Miscellaneous	DataVal
QC.O05	DVSAMP		CHAR	10	Sample Id	DataVal
QC.O06	DVCOM	(3)	CHAR	60	Blind QC comments	DataVal

LOVE CANAL HABITABILITY STUDY

QUALITY CONTROL MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
QC.009	QCSURRA		CHAR	1	Check surrogates spiked into all samples	DataVal
QC.010	QCSURRB		CHAR	1	Recoveries within criteria	DataVal
QC.011	QCSURRC		CHAR	1	Miscellaneous	DataVal
QC.012	QCSURCM	(3)	CHAR	60	Surrogates Comments	DataVal
QC.015	QCINTA		CHAR	1	Internal Standards RT Criteria	DataVal
QC.016	QCINTB		CHAR	1	Internal Standards Area Criteria	DataVal
QC.017	QCINTC		CHAR	1	Internal Standards Miscellaneous	DataVal
QC.018	QCINTCM	(3)	CHAR	60	Internal Standards Comments	DataVal
QC.021	QCIDA		CHAR	1	Id All ions maximize simultaneously	DataVal
QC.022	QCIDB		CHAR	1	Id Appropriate flags used	DataVal
QC.023	QCIDC		CHAR	1	Id All peaks reported that meet Id criteria	DataVal
QC.024	QCIDD		CHAR	2	Id Low level peaks examined	DataVal
QC.025	QCIDE		CHAR	2	Id Miscellaneous	DataVal
QC.026	QCIDCOM	(3)	CHAR	60	Id Comments	DataVal
QC.029	QCQTA		CHAR	1	Quantitation Appropriate RRF's used if nonstandard	DataVal
QC.030	QCQTB		CHAR	1	Quantitation Check integration parameters if manual	DataVal
QC.031	QCQTC		CHAR	2	Quantitation Miscellaneous	DataVal
QC.032	QCQTCOM	(3)	CHAR	60	Quantitation Comments	DataVal
QC.035	QCGENA		CHAR	2	General Review case narrative and address all problems	DataVal
QC.036	QCGENB		CHAR	2	Examine SICPS	DataVal
QC.037	QCGENC		CHAR	2	Examine quantitation reports	DataVal
QC.038	QCGEND		CHAR	2	Miscellaneous	DataVal
QC.039	QCGENCM	(3)	CHAR	60	General Comments	DataVal
QC.042	QCDQ	(8,5)	CHAR	2	Data Qualifiers 8 Analytes by 5 samples	DataVal

******* Integrated DB Audit System Flags **********						
QC.P01	QCF1FLAG		CHAR	1	Flag for Form1 Match Results Values: 1 = Found Form1 and all data matches 2 = Found Form1 and some data does not match 3 = Form1 not found	IntDBBld
QC.P02	QCRECALC		CHAR	1	Flag for calculation descrepancies Values: * = descrepancy found in calculation blank = no descrepancy found in calculation	IntDBBld

LOVE CANAL HABITABILITY STUDY

QUALITY CONTROL ANCILLARY FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
******* Keys *******						
QA.A01	QCANALID		CHAR	23	QC Lab Analysis Id - (Lab Id + Lab Analysis Id)	LabData
******* Data Transfer Tracking *******						
QA.B01	QCGENDTE		NUM	8	LabData Gen Date	LabData
QA.B02	QCGENTME		NUM	8	LabData Gen Time	LabData
QA.B03	QCADDDTE		NUM	8	DB Add Date	IntDBBld
QA.B04	QCADDTME		NUM	8	DB Add Time	IntDBBld
QA.B05	QCUPDDTE		NUM	8	DB Most Recent Update Date	IntDBBld
QA.B06	QCUPDTME		NUM	8	DB Most Recent Update Time	IntDBBld
QA.B07	QCUPDCNT		NUM	8	DB Update Count	IntDBBld
******* Data Replaced by Corrections *******						
QA.C01	QCLCA	(8,3)	NUM	8	Area, by 8 LCICs, by 3 Ions	LabData
QA.C02	QCLCS	(8,3)	NUM	8	Scan, by 8 LCICs, by 3 Ions	LabData
QA.C03	QCLCR	(8,3)	NUM	8	Retention Time, by 8 LCICs, by 3 Ions	LabData
QA.C04	QCISA	(5)	NUM	8	Area, by 5 Int. Stds. (Primary Ion)	LabData
QA.C05	QCPYRA		NUM	8	Area Pyrene-D10 (Secondary Ion)	LabData
QA.C06	QCISS	(5)	NUM	8	Scan, by 5 Int. Stds. (Primary Ion)	LabData
QA.C07	QCPYRS		NUM	8	Scan Pyrene-D10 (Secondary Ion)	LabData
QA.C08	QCISR	(5)	NUM	8	Retention Time, by 5 Int. Stds. (Primary Ion)	LabData
QA.C09	QCPYRR		NUM	8	Retention Time Pyrene-D10 (Secondary Ion)	LabData
QA.C10	QCSSA	(3)	NUM	8	Area, by 3 Surrogates (Primary Ion)	LabData
QA.C11	QCSSS	(3)	NUM	8	Scan, by 3 Surrogates (Primary Ion)	LabData
QA.C12	QCSSR	(3)	NUM	8	Retention Time, by 3 Surrogates (Primary Ion)	LabData

6.0 Form I Master File

The FORM I Master File contains a record for each validated Form I generated by the analytic laboratories. A Form I was generated for each QC sample and for each field sample that was collected, prepared, and sent to the analytic laboratories. Figure 6-1 depicts the record set relationship among the Field Sample, QC Sample, and Form I Master Files.

The data on the Form I, plus the validation results generated by EMSL-LV, were separately keyed, verified, and loaded into this file. As such, these are the "official, approved, validated" results. The "same" data was also loaded into the other master files in the data base from the LabData Systems in each analytic laboratory. Along with the concentrations, all the background and QC data that go into computing the concentration results were loaded. Since there were changes and re-submissions required of the analysis laboratories during the validation process, some discrepancies resulted between the Form I data that were keyed and loaded into the FORM I file and the data taken from the LabData System and loaded into the other files. The discrepancies appear to be the result of earlier versions of the quantitation report data being included in the data taken from the LabData systems in the laboratories. During the data validation process, there was a substantial number of re-submissions generated by the laboratories. The resulting occurrence of multiple versions of data seems to have caused the problem. In all cases, where a discrepancy exists between the data from LabData and the data from the Form I, the Form I data is correct. The audit results fields should be referred to in order to determine if any discrepancies exist.

When working with the analysis results, it should be noted that each sample was analyzed for the presence of eight analytes, i.e., the LCICs. Data usability flags are assigned to each analyte within a sample (LCICUSE1- LCICUSE8). Thus, the usability of each analyte must be examined separately. For the meaning of the usability flags, refer to the field descriptions in Section 6.3. Refer to Volume III, Soil Assessment--Indicator Chemicals, Appendix H, CH2M HILL, 1988, for a complete explanation of validation flags associated with a usability flag of "UNCERTAIN" or "BAD."

It should also be noted that there are duplicate field sample analyses present. The statistical analyses were performed using only the analysis selected by the project chemists as the most appropriate. For information on creating the data subset used for the primary statistical comparisons, see Section 8.6.

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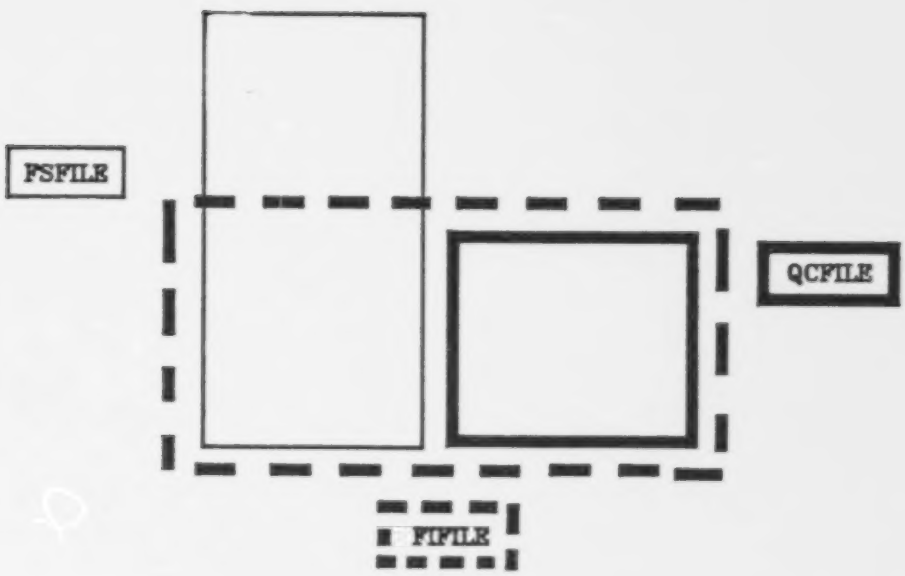

Figure 6-1
Record Set Relationships

6.1 Logical Record Description

A logical record in this file contains data for each Form I validated by EMSL-LV. The data elements are organized in groups, as follows:

- KEYS AND STATUS - the primary, unique identifier of each record in the file, along with any other (perhaps non-unique) keys, and the status flag.

- SAMPLE INFORMATION - the data related to samples login, sample extraction, and GC/MS injection.

- SUMMARY SAMPLE DATA VALIDATION QUALIFIERS - flags that summarize, by analyte, the data usability flags assigned by EMSL-LV (these flags were assigned at either the sample level or the analyte level). If a sample was flagged as "UNCERTAIN" solely based on holding time, it was re-classified as "GOOD."

- SAMPLE SPECIFIC DATA VALIDATION QUALIFIERS - qualifiers at the sample level, denoting data validation deficiencies.

- ANALYTE SPECIFIC LABDATA AND LABORATORY QUALIFIERS - qualifiers at the analyte level, denoting anomalies in the data and identifying data quality deficiencies.

- ANALYTE SPECIFIC FLAGS - flags relating to presence of ions, scan range, ion ratio, and relative retention time.

- FORM 1 COMMENTS - textual explanation of any modifications made to the quantitation results using the LabData system.

- INTEGRATED DATA BASE AUDIT SYSTEM FLAGS - results of the automated audits and validations performed during the data base building process.

6.2 Logical Subsets of the File - Special Screening

The primary grouping of logical subsets in the FORM I Master File is based upon sample types. The table below presents these sample types and discusses sub-groups within each sample type.

Sample Type Code (F1TYPE)	Description
HS	The field samples. These samples' results were used for the comparison analyses to determine if

any differences in contamination levels existed between the Love Canal Emergency Declaration Area (EDA) and the comparison areas. The actual statistical analyses were performed using the "GOOD," non-duplicate subset of this data.

SPLIT — The field split half of a field sample was separated for inter- and intra-laboratory comparison of performance. The field sample half retained the originally assigned project sample ID, and the field split half was assigned a different project sample ID.

FHB — Field handling blanks were actually Quality Control (QC) samples that were sent to the analytic laboratories just as field samples were (i.e., they were "blind"). They had a similar appearance and soil composition as field samples but were known to contain no detectable concentrations of LCICs. They were analyzed and handled just as field samples were, and the results indicated whether or not any contamination had been introduced by the analytic laboratory.

PHB — Preparation Handling Blanks were actually QC samples introduced at the sample preparation laboratory and sent to analytic laboratories just as field samples were sent (i.e., they were "blind"). They were analyzed and reported just as field samples were, and the results indicated whether any contamination was introduced by the preparation laboratory.

HT — Holding time samples were soil samples used to study the effects of extending the holding time on LCIC concentrations in the sample. QCEMSL EMSL Blind QC samples were samples spiked with known concentrations of LCICs, but the levels were not known by the analytic laboratory. A Blind QC sample was extracted with each extraction batch of samples and analyzed. If a given level of recovery was not achieved in the Blind QC, then the laboratory re-extracted and re-analyzed the field samples in the extraction batch.

MS — The Matrix Spike and Matrix Spike Duplicate samples (MSD) were created by splitting every twentieth field sample into three parts. One-third was treated as a normal field sample (i.e., the "native" sample in a native/MS/MSD set of analyses), one-third as an MS analysis, and one-third as the MSD. Each MS and MSD was then spiked with a fixed amount of LCICs. The results were then used for QC purposes. See Section 8.5 for a

description of how to merge the native samples, with MS/MSD analyses.

BL — This group includes both Reagent or Instrument blanks as well as Method Blanks. The Method Blank is a blank sample, prepared by the analytic laboratory, containing no known levels of LCICs. This sample was then extracted in a batch of field samples, subjected to the same handling and storage and analyzed with the field samples. The Reagent Blank is also a blank sample, made from the solvents used during the sample extraction process and analyzed to determine if the analysis process was introducing LCIC contamination into the field samples.

6.3 Data Element Dictionary

The data element dictionary for the Form I Master File follows this page.

LOVE CANAL HABITABILITY STUDY
FORM I MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
******* Keys and Status *******						
F1.A01	F1ANALID		CHAR	20	Analysis Lab Sample Id (Lab Id + Lab Analysis Id)	LabData
F1.A02	CLEANHS		CHAR	10	Original Project ID (HS Number)	LabData
******* Sample Information *******						
F1.B01	F1SMPL		CHAR	10	Project Sample Field Id (HS #)	LabData
F1.B02	F1TYPE		CHAR	6	Type of sample Values: MS = Matrix Spike MSD = Matrix Spike Duplicate BL = Method Blank or Reagent Blank QCEMSL = EMSL Blind QC Sample HS = Field Sample HS REP= Field Sample Replacement HT = Holding Time Blank FHB = Field Handling Blank PHB = Prep Lab Handling Blank SPLIT = Field Split SSB = Shipping and Storage Blank SSB SP = Shipping and Storage Blank Split	LabData
F1.B03	F1GENDTE		CHAR	8	LabData Generation Date	LabData
F1.B04	F1GENTME		CHAR	8	LabData Generation Time	LabData
F1.B05	F1LDVER		CHAR	5	LabData Software Version	LabData
F1.B06	F1MOIST		NUM	8	Percent Moisture	LabData
F1.B07	F1PRESCR		CHAR	3	Flag for Analysis Pre-screen Values: MS = GC/MS pre-screen performed ECD = GC/ECD pre-screen performed blank = pre-screen not performed	LabData
F1.B08	F1SULFUR		CHAR	1	Flag for Sulphur Cleanup Performed Values: blank or N = sulphur cleanup not performed Y = sulphur cleanup performed	LabData
F1.B09	F1ANLST		CHAR	8	GC/MS Analyst	LabData
F1.B10	F1WTEXT		NUM	8	Weight Extracted	LabData
F1.B11	F1AADTE		CHAR	8	Analysis Date	LabData
F1.B12	F1AATME		CHAR	8	Analysis Time	LabData
F1.B13	F1CONCD		NUM	8	Concentration Dilution Factor	LabData
F1.B14	F1QFILE		CHAR	12	GC/MS Shift Results File Name	LabData
F1.B15	F1DFILE		CHAR	15	GC/MS Data File Id	LabData

LOVE CANAL HABITABILITY STUDY
FORM I MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
******* Summary Sample Data Validation Qualifiers **********						
F1.C01	LCICUSE	(8)	CHAR	2	Data validation usability flags, by 8 LCICs Values: 'G ' = Good; no QC flaws. 'U ' = Uncertain; minor QC flaws;may or may not be usable, depending on application. 'B ' = Bad; major QC flaws; data unusable.	IntDBBld
******* EMSL-LV Sample Specific Data Validation Qualifiers **********						
F1.D01	S_FLAG	(4)	CHAR	2	Sample specific qualifiers (1 through 4) Values: E1-E8 M1-M4 I2-I5 B1-B4 Q1-Q8 QA Z1-Z9 ZA-ZJ H1-H4 K2 (See Volume III, Soil Assessment Indicator Chemicals, Appendix H, CH2M Hill 1988 for a full description of these qualifiers.)	Form1DE
F1.D05	S_FLAG5		CHAR	2	Sample specific qualifier 5 - EMSL-LV data validation rating Values: blank = usability is flagged on an analyte basis (see next data group) 'G ' = Good; no QC flaws. 'U ' = Uncertain; minor QC flaws;may or may not be usable, depending on application. 'B ' = Bad; major QC flaws; data unusable.	Form1DE
******* Analyte Specific LabData and Laboratory Qualifiers **********						
					Values for E_FLAGnA through E_FLAGnD: E1-E8 M1-M4 I2-I5 B1-B4 Q1-Q8 QA Z1-Z9 ZA-ZJ H1-H4 K2 Values for E_FLAGnE (analyte usability): 'G ' = Good; no QC flaws. 'U ' = Uncertain; minor QC flaws;may or may not be usable, depending on application. 'B ' = Bad; major QC flaws; data unusable. blank = this flag slot not used (See Volume III, Soil Assessment Indicator Chemicals, Appendix H, CH2M Hill 1988 for a full description of these qualifiers.)	
F1.E01	E_FLAG1A		CHAR	2	1,2-Dichlorobenzene qualifier A	Form1DE
F1.E02	E_FLAG1B		CHAR	2	1,2-Dichlorobenzene qualifier B	Form1DE
F1.E03	E_FLAG1C		CHAR	2	1,2-Dichlorobenzene qualifier C	Form1DE
F1.E04	E_FLAG1D		CHAR	2	1,2-Dichlorobenzene qualifier D	Form1DE
F1.E05	E_FLAG1E		CHAR	2	1,2-Dichlorobenzene qualifier E	Form1DE
F1.E06	E_FLAG2A		CHAR	2	1,2,4-Trichlorobenzene qualifier A	Form1DE
F1.E07	E_FLAG2B		CHAR	2	1,2,4-Trichlorobenzene qualifier B	Form1DE
F1.E08	E_FLAG2C		CHAR	2	1,2,4-Trichlorobenzene qualifier C	Form1DE
F1.E09	E_FLAG2D		CHAR	2	1,2,4-Trichlorobenzene qualifier D	Form1DE

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FORM I MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
F1.E10	E_FLAG2E		CHAR	2	1,2,4-Trichlorobenzene qualifier E	Form1DE
F1.E11	E_FLAG3A		CHAR	2	1,2,3,4-Tetrachlorobenzene qualifier A	Form1DE
F1.E12	E_FLAG3B		CHAR	2	1,2,3,4-Tetrachlorobenzene qualifier B	Form1DE
F1.E13	E_FLAG3C		CHAR	2	1,2,3,4-Tetrachlorobenzene qualifier C	Form1DE
F1.E14	E_FLAG3D		CHAR	2	1,2,3,4-Tetrachlorobenzene qualifier D	Form1DE
F1.E15	E_FLAG3E		CHAR	2	1,2,3,4-Tetrachlorobenzene qualifier E	Form1DE
F1.E16	E_FLAG4A		CHAR	2	2-Chloronaphthalene qualifier A	Form1DE
F1.E17	E_FLAG4B		CHAR	2	2-Chloronaphthalene qualifier B	Form1DE
F1.E18	E_FLAG4C		CHAR	2	2-Chloronaphthalene qualifier C	Form1DE
F1.E19	E_FLAG4D		CHAR	2	2-Chloronaphthalene qualifier D	Form1DE
F1.E20	E_FLAG4E		CHAR	2	2-Chloronaphthalene qualifier E	Form1DE
F1.E21	E_FLAG5A		CHAR	2	Alpha-BHC qualifier A	Form1DE
F1.E22	E_FLAG5B		CHAR	2	Alpha-BHC qualifier B	Form1DE
F1.E23	E_FLAG5C		CHAR	2	Alpha-BHC qualifier C	Form1DE
F1.E24	E_FLAG5D		CHAR	2	Alpha-BHC qualifier D	Form1DE
F1.E25	E_FLAG5E		CHAR	2	Alpha-BHC qualifier E	Form1DE
F1.E26	E_FLAG6A		CHAR	2	Delta-BHC qualifier A	Form1DE
F1.E27	E_FLAG6B		CHAR	2	Delta-BHC qualifier B	Form1DE
F1.E28	E_FLAG6C		CHAR	2	Delta-BHC qualifier C	Form1DE
F1.E29	E_FLAG6D		CHAR	2	Delta-BHC qualifier D	Form1DE
F1.E30	E_FLAG6E		CHAR	2	Delta-BHC qualifier E	Form1DE
F1.E31	E_FLAG7A		CHAR	2	Beta-BHC qualifier A	Form1DE
F1.E32	E_FLAG7B		CHAR	2	Beta-BHC qualifier B	Form1DE
F1.E33	E_FLAG7C		CHAR	2	Beta-BHC qualifier C	Form1DE
F1.E34	E_FLAG7D		CHAR	2	Beta-BHC qualifier D	Form1DE
F1.E35	E_FLAG7E		CHAR	2	Beta-BHC qualifier E	Form1DE
F1.E36	E_FLAG8A		CHAR	2	Gamma-BHC qualifier A	Form1DE
F1.E37	E_FLAG8B		CHAR	2	Gamma-BHC qualifier B	Form1DE
F1.E38	E_FLAG8C		CHAR	2	Gamma-BHC qualifier C	Form1DE
F1.E39	E_FLAG8D		CHAR	2	Gamma-BHC qualifier D	Form1DE
F1.E40	E_FLAG8E		CHAR	2	Gamma-BHC qualifier E	Form1DE
F1.E41	CONC	(8)	NUM	8	Concentrations, by LCIC Order of the LCICs: 1,2-Dichlorobenzene 1,2,4-Trichlorobenzene 1,2,3,4-Tetrachorobenzene 2-Chloronaphthalene Alpha-BHC Delta-BHC Beta-BHC Gamma-BHC	LabData
F1.E42	EXT_DATE		CHAR	8	Date Sample Extracted	Form1DE

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FORM I MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
******* Analyte Specific Flags *******						
F1.F01	ALLIONS	(8)	CHAR	1	All Ions Flags, by 8 LCICs Values: blank = all three ions present '*' = one or more ions missing	LabData
F1.F02	SCANRNG	(8)	CHAR	1	Scan Range Flags, by 8 LCICs Values: blank = scan range less than or equal to 2 '*' = scan range greater than 2	LabData
F1.F03	IONRATI	(8)	CHAR	1	Ion Ratio Flags Values: blank = ion ratio within 20% of theoretical '*' = ion ratio greater than 40 % from theoretical '+' = ion ratio between 20% and 40% from theoretical	LabData
F1.F04	RRT	(8)	CHAR	1	Relative Retention Time Flags Values: blank = within the relative retention time window '*' = outside of relative retention time window	LabData
******* Form 1 Comments *******						
F1.G01	COMM	(10)	CHAR	80	Form 1 Comments - containing explanation of manual LabData quantitation override	LabData
******* Integrated DB Audit System Results *******						
F1.H01	F1TRACK		CHAR	1	Sample not found in Sample Tracking Values: * = not found in Sample Tracking blank = found in Sample Tracking	IntDBBld

7.0 Blind Quality Control (QC) Spike Master File

In the Blind QC Spike Master File, a record contains analyte spiking levels for a blind QC sample sent by EMSL-LV to an analytical laboratory.

7.1 Logical Record Description

The data elements in a logical record are organized in data groups, as follows:

- KEYS - the primary, unique identifier of each record in the file.

- BLIND QUALITY CONTROL SPIKE INFORMATION - information on spike levels, by analyte, along with the specific bottle number.

7.2 Logical Subsets of the File - Special Screening

This file does not contain any data elements that define logical subsetting.

7.3 Data Element Dictionary

The data element dictionary for the Blind Quality Control Master File follows this page.

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LOVE CANAL HABITABILITY STUDY

BLIND QUALITY CONTROL MASTER FILE - DATA ELEMENT DICTIONARY

DATA ELEMENT ID	NAME	ARRAY	TYPE	LENGTH	DESCRIPTION	SOURCE
******* Key **********						
BQ.A01	QCSMPL		CHAR	8	Sample Id	BlindQC
******* Analyte Spiking Level Data **********						
BQ.B01	QCBOTTLE		CHAR	3	Bottle Number	BlindQC
BQ.B02	QCSPIKE	(8)	NUM	8	Spike Levels, by 8 LCICs in ppb	BlindQC

8.0 Combining Files

Since the Data Base is composed of ten files, some data analyses may require combining two or more of these files. This is accomplished through SAS by a series of steps that usually involves sorting the records and then combining or merging the files based on one of the keys they contain.

The first four subsections present outlines of the basic steps needed to complete some common file combinations. The last two subsections contain the actual SAS code used during two of the data analyses.

8.1 Form I with Detailed Data

To combine the "official" analytical results in the Form I records (F1FILE) with detail data in the sample master files (FSFILE and QCFILE), the following steps must be taken:

1. sort F1FILE on F1ANALID
2. concatenate F1FILE and QCFILE, renaming QCANALID and ALANALID to F1ANALID
3. sort output of step 2. by F1ANALID
4. merge F1FILE and output of step 3. by F1ANALID, retaining only observations that are in both files

8.2 Field Samples with Calibration Records

To combine field samples (FSFILE) with continuing calibration (CCFILE)and initial calibration (ICFILE) records, the following steps must be taken:

1. select desired FSFILE records (by FSTYPE or other criteria, if any)
2. sort output of step 1. by CCANALID
3. sort CCFILE by CCANALID
4. merge the output of step 2. and step 3. by CCANALID, retaining only observations that are in both files
5. sort ICFILE by ICANALID
6. merge output of step 4. with output of step 5. by ICANALID, retaining only observations that are in both files

8.3 Field Samples with Method Blanks

To combine field samples with their associated method blanks, the following steps must be taken:

1. select QCFILE records with QCTYPE = "BLM", renaming QCANALID to MBANALID
2. sort output of step 1. on MBANALID
3. select FSFILE records (as desired)
4. sort output of step 3. on MBANALID
5. merge output of step 2. and output of step 4. by MBANALID, retaining only observations that are in both files

8.4 Blind QC Results with Spiking Levels

The merging of blind QC results with blind QC spiking levels is accomplished by doing the following:

1. select F1FILE records whose F1TYPE = "QCEM"
2. sort output of step 1. on F1ANALID
3. select QCFILE records whose QCTYPE = "QCEM", renaming QCANALID to F1ANALID
4. sort output of step 3. on F1ANALID
5. merge output of step 2. and output of step 4. by F1ANALID, retaining only observations that are in both files
6. sort output of step 5. by CLEANHS
7. read BQFILE, renaming QCSMPL to CLEANHS
8. sort output of step 7. by CLEANHS
9. merge the output of step 6. and the output of step 8. by CLEANHS, retaining only observations that are in both files

8.5 Native Field Sample MS/MSD Sets

An example of the SAS code necessary to create the native field sample MS/MSD sets is as follows:

```
DATA FS;
  SET VAXDB1.F1FSFILE;
  LENGTH MSSAMP $ 8 LAB $ 3;
  ARRAY FSCONCB(8) FSCONCB1-FSCONCB8;
  ARRAY FSRRF(8) FSRRF1-FSRRF8;
  ARRAY FSCONC(8) FSCONC1-FSCONC8;
  J = INDEX(FSSMPL,'MS');
  IF FSALID='AQI' THEN LABID=1;
  IF FSALID='CEC' THEN LABID=2;
  IF FSALID='VER' THEN LABID=3;
  IF FSALID='NUS' THEN LABID=4;
  IF FSALID='EMS' THEN LABID=5;
  IF FSALID='MGM' THEN LABID=6;
  IF FSALID='CAA' THEN LABID=7;
  K = 10 - J + 1;
  MSSAMP = SUBSTR(FSSMPL,J,K);
  DO I = 1 TO 8;
    FSCONC(I) = 0;
    IF FSRRF(I)=' ' THEN FSCONC(I)=FSCONCB(I) * (100-FSMOIST)/100;
    END;
  KEEP MSSAMP ALANALID CLEANHS FSCONC1-FSCONC8 LABID LAB;
PROC SORT DATA=FS; BY MSSAMP;

DATA MS;
  SET VAXDB1.QCFILE;
  LENGTH MSSAMP $8 MSLAB $ 3;
  ARRAY QCCONCB(8) QCCONCB1-QCCONCB8;
  ARRAY MSCONC(8) MSCONC1-MSCONC8;
  IF INDEX(QCSMPL,'MS')>0 AND INDEX(QCSMPL,'EM')=0 AND
     INDEX(QCSMPL,'MSD')=0;
  J = INDEX(QCSMPL,'MS') + 2;
  K = 10 - J + 1;
  MSSAMP = SUBSTR(QCSMPL,J,K);
  MSCADD = 5 * 20 / QCWTEXT;
  DO I = 1 TO 8;
    MSCONC(I) = QCCONCB(I) * (100-QCMOIST)/100;
    END;
  KEEP QCSMPL QCALID MSSAMP MSCADD MSCONC1-MSCONC8 QCSPRCU1-QCSPRCU8
     - QCSPRCL1-QCSPRCL8 QCSPRL1-QCSPRL8;
PROC SORT DATA=MS; BY MSSAMP;

DATA MSD;
  SET VAXDB1.QCFILE;
  LENGTH MSSAMP $8 MSDLAB $ 3;
  ARRAY QCCONCB(8) QCCONCB1-QCCONCB8;
  ARRAY MSDCONC(8) MSDCONC1-MSDCONC8;
  IF INDEX(QCSMPL,'MSD')>0 AND INDEX(QCSMPL,'EM')=0;
  J = INDEX(QCSMPL,'MSD') + 3;
  K = 10 - J + 1;
```

```
  MSSAMP = SUBSTR(QCSMPL,J,K);
  MSDCADD = 5 * 20 / QCWTEXT;
  DO I = 1 TO 8;
    MSDCONC(I) = QCCONCB(I) * (100-QCMOIST)/100;
    END;
  KEEP QCSMPL QCALID MSSAMP MSDCADD MSDCONC1-MSDCONC8;
PROC SORT DATA=MSD; BY MSSAMP;

DATA MRGMSMSD ERRMS MRG2MS MRG3MS;
  ARRAY MSCONC(8) MSCONC1-MSCONC8;
  ARRAY MSDCONC(8) MSDCONC1-MSDCONC8;
  ARRAY FSCONC(8) FSCONC1-FSCONC8;
  ARRAY MSPR(8) MSPR1-MSPR8;
  ARRAY MSDPR(8) MSDPR1-MSDPR8;
  ARRAY MSRPD(8) MSRPD1-MSRPD8;
  ARRAY QCSPRCU(8) QCSPRCU1-QCSPRCU8;
  ARRAY QCSPRCL(8) QCSPRCL1-QCSPRCL8;
  ARRAY QCSPRL(8) QCSPRL1-QCSPRL8;

  MERGE FS(IN=INFS) MS(IN=INMS) MSD(IN=INMSD);
  BY MSSAMP;
  IF INFS AND (INMS OR INMSD);
  IF NOT FIRST.MSSAMP AND NOT LAST.MSSAMP THEN OUTPUT ERRMS;
  ELSE DO;
  INTFLAG = 1;
  DO I = 1 TO 8;
    MSPR(I) = (MSCONC(I)-FSCONC(I))/MSCADD*100;
    MSDPR(I) = (MSDCONC(I)-FSCONC(I))/MSDCADD*100;
    LCIC = I;
    LOWLIM = QCSPRCL(I); UPLIM = QCSPRCU(I);
    MS2PR = MSPR(I);
    OUTPUT MRG2MS;
    MS2PR = MSDPR(I);
    OUTPUT MRG2MS;
    MSRPD(I) = ABS(MSPR(I)-MSDPR(I))/(MSPR(I)+MSDPR(I))*200;
    UPLIM= QCSPRCL(I); LOWLIM=0.;
    MS2RPD = MSRPD(I);
    OUTPUT MRG3MS;
    END;
  OUTPUT MRGMSMSD;
  END;
```

8.6 Creating the Subset Used for Statistical Analysis

The SAS code used to create the subset of data used for statistical analysis is as follows:

```
DATA F1FILE;
SET VAXDB1.FORM1;
KEEP ANALID;
LENGTH ANALID $ 20;
ANALID=F1ANALID;
IF ANALID EQ "CAA8711125-01AS" THEN DELETE;
IF ANALID EQ "MGMLC09974R03  " THEN DELETE;
IF ANALID EQ "VER41283       " THEN DELETE;
IF ANALID EQ "EMSREHS0219    " THEN DELETE;
IF ANALID EQ "EMSREHS0253    " THEN DELETE;
IF ANALID EQ "EMSHS0344      " THEN DELETE;
IF ANALID EQ "VER40438RE     " THEN DELETE;
IF ANALID EQ "VER40075       " THEN DELETE;
IF ANALID EQ "MGMLC09976T01  " THEN DELETE;
IF ANALID EQ "MGMLC10005R08  " THEN DELETE;
IF ANALID EQ "EMSHS0661      " THEN DELETE;
IF ANALID EQ "EMSHS0771      " THEN DELETE;
IF ANALID EQ "MGMLC10020R8   " THEN DELETE;
IF ANALID EQ "MGMLC09974007  " THEN DELETE;
IF ANALID EQ "EMSREHS1315    " THEN DELETE;
IF ANALID EQ "CEC587799      " THEN DELETE;
IF ANALID EQ "AQ17855412     " THEN DELETE;
IF ANALID EQ "AQ177390E2     " THEN DELETE;
IF ANALID EQ "CAA8710222-01T " THEN DELETE;
IF ANALID EQ "CAA8710222-02SRE" THEN DELETE;
IF ANALID EQ "AQ17886112     " THEN DELETE;
IF ANALID EQ "AQ177393E2     " THEN DELETE;
IF ANALID EQ "VER41364RE     " THEN DELETE;
IF ANALID EQ "MGMLC09974002  " THEN DELETE;

PROC SORT DATA=F1FILE;
  BY ANALID;

DATA FSFILE;
  SET VAXDB1.FSFILE;
  IF NEIGHID > 0 AND SUBSTR(SAMPTYPE,1,2) = 'HS';
  ALANALID=LEFT(ALANALID);
  ANALID=ALANALID;

PROC SORT DATA=FSFILE;
  BY ANALID;

DATA VAXDB1.F1FSFILE;
    MERGE F1FILE (IN=INF1) FSFILE (IN=INFS);
    BY ANALID;
    IF INF1 AND INFS;
```

APPENDIX A

Data Element Name Index

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DATA ELEMENT NAME INDEX

Data Element ID = column heading.cell contents (e.g. BQ.B01)

Data Element Name	FS	FA	IC	IA	CC	CA	QC	QA	F1	BQ
ALANALID	A01	A01								
ALLIONS									F01	
ALRECBY	H04									
AREAID	F12									
CBOTTLE										B01
CCAADTE					B01					
CCAATME					B02					
CCADDDTE					C03	B03				
CCADDTME					C04	B04				
CCALID					D02					
CCANALID	B02				A01	A01				
CCANLST					E02					
CCCANAL					G03					
CCCDATE					G01					
CCCISA					G07					
CCCISR					G09					
CCCISS					G08					
CCCLCA					G04					
CCCLCR					G06					
CCCLCS					G05					
CCCPYRA					G10					
CCCPYRR					G12					
CCCPYRS					G11					
CCCSSA					G13					
CCCSSR					G15					
CCCSSS					G14					
CCCTIME					G02					
CCFILE					E03					
CCGENDTE					C01	B01				
CCGENTME					C02	B02				
CCHISR					F11					
CCHISS					F10					
CCHLCR					F09					
CCHLCS					F08					
CCHPYRR					F13					
CCHPYRS					F12					
CCHSSR					F15					
CCHSSS					F14					
CCINJVL					E04					
CCINSTID					E01					
CCISA					H04	C04				
CCISPH					F05					
CCISR					H08	C08				
CCISS					H06	C06				

DATA ELEMENT NAME INDEX

Data Element ID = column heading.cell contents (e.g. BQ.B01)

Data Element Name	FS	FA	IC	IA	CC	CA	QC	QA	F1	BQ
CCLCA					H01	C01				
CCLCPH					F04					
CCLCR					H03	C03				
CCLCS					H02	C02				
CCPC2ID					A02					
CCPDC					I05					
CCPDF					I06					
CCPDOUT					I07					
CCPDRF					I04					
CCPYRA					H05	C05				
CCPYRPH					F06					
CCPYRR					H09	C09				
CCPYRS					H07	C07				
CCQFILE					F01					
CCQION					F03					
CCQMTH					F02					
CCRECALC					L01					
CCRFA					I01					
CCRFPH					I02					
CCRIR					I03					
CCRR					I08					
CCSMPL					D01					
CCSSA					H10	C10				
CCSSPH					F07					
CCSSR					H12	C12				
CCSSS					H11	C11				
CCSTATUS					A03					
CCUPDCNT					C07	B07				
CCUPDDTE					C05	B05				
CCUPDTME					C06	B06				
CLEANHS	B08						A03		A02	
COLFORM	F01									
COLFORMR	F02									
COLLECTR	F15									
COLMLEN	F18									
COMM									G01	
CONC									E41	
CSMPL										A01
CSPIKE										B02
DUPLICAT	F19									
DVCCCALA					K30					
DVCCCALB					K31					
DVCCCALC					K32					
DVCCCOM					K35					
DVCCDT					K33					

DATA ELEMENT NAME INDEX

Data Element ID = column heading.cell contents (e.g. BQ.B01)

Data Element Name	FS	FA	IC	IA	CC	CA	QC	QA	F1	BQ
DVCCTM					K34					
DVCHKA							O01			
DVCHKB							O02			
DVCHKC							O03			
DVCHKD							O04			
DVCOM							O06			
DVDELIV					K01					
DVEPAA					K24					
DVEPAB					K25					
DVEPAC					K26					
DVEPACM					K29					
DVEPAD					K27					
DVEPASMP					K28					
DVHALF					K13					
DVMISS					K02					
DVPC1A					K04					
DVPC1B					K05					
DVPC1C					K06					
DVPC1CM					K14					
DVPC1D					K07					
DVPC1DT					K10					
DVPC1E					K08					
DVPC1F					K09					
DVPC1TM					K11					
DVPC2A					K15					
DVPC2B					K16					
DVPC2C					K17					
DVPC2CM					K23					
DVPC2D					K18					
DVPC2DT					K21					
DVPC2E					K19					
DVPC2F					K20					
DVPC2TM					K22					
DVPCMDP					K12					
DVRES					K03					
DVSAMP							O05			
EXCPFLAG	G21									
EXT_DATE									E42	
E_FLAG1A									E01	
E_FLAG1B									E02	
E_FLAG1C									E03	
E_FLAG1D									E04	
E_FLAG1E									E05	
E_FLAG2A									E06	
E_FLAG2B									E07	

DATA ELEMENT NAME INDEX

Data Element ID = column heading.cell contents (e.g. BQ.B01)

Data Element Name	FS	FA	IC	IA	CC	CA	QC	QA	F1	BQ
E_FLAG2C									E08	
E_FLAG2D									E09	
E_FLAG2E									E10	
E_FLAG3A									E11	
E_FLAG3B									E12	
E_FLAG3D									E14	
E_FLAG3E									E15	
E_FLAG4A									E16	
E_FLAG4B									E17	
E_FLAG4C									E18	
E_FLAG4D									E19	
E_FLAG4E									E20	
E_FLAG5A									E21	
E_FLAG5B									E22	
E_FLAG5C									E23	
E_FLAG5D									E24	
E_FLAG5E									E25	
E_FLAG6A									E26	
E_FLAG6B									E27	
E_FLAG6C									E28	
E_FLAG6D									E29	
E_FLAG6E									E30	
E_FLAG7A									E31	
E_FLAG7B									E32	
E_FLAG7C									E33	
E_FLAG7D									E34	
E_FLAG7E									E35	
E_FLAG8A									E36	
E_FLAG8B									E37	
E_FLAG8C									E38	
E_FLAG8D									E39	
E_FLAG8E									E40	
F1AADTE									B11	
F1AATME									B12	
F1ANALID									A01	
F1ANLST									B09	
F1CONCD									B13	
F1DFILE									B15	
F1GENDTE									B03	
F1GENTME									B04	
F1LDVER									B05	
F1MOIST									B06	
F1PRESCR									B07	
F1QFILE									B14	
F1SMPL									B01	

DATA ELEMENT NAME INDEX

Data Element ID = column heading.cell contents (e.g. BQ.B01)

Data Element Name	FS	FA	IC	IA	CC	CA	QC	QA	F1	BQ
F1SULFUR									B08	
F1TRACK									H01	
F1TYPE									B02	
F1WTEXT									B10	
FCOCFORM	F21									
FDUPID	C02									
FHBID	C03									
FLDCOM	F20									
FLFEDEX	F23									
FLPRVBLK	F25									
FLSRMKS	F24									
FSAADTE	D11									
FSAATME	D12									
FSAD	P03									
FSADCL	P07									
FSADCU	P08									
FSADDDTE	E03	B03								
FSADDTME	E04	B04								
FSAEDTE	D10									
FSAF	P05									
FSALCOND	H03									
FSALDTEL	D09									
FSALDTES	D08									
FSALID	H02									
FSANLST	J02									
FSCANAL	L03									
FSCCREF	R04									
FSCDATE	L01									
FSCISA	L07									
FSCISR	L09									
FSCISS	L08									
FSCLCA	L04									
FSCLCR	L06									
FSCLCS	L05									
FSCONCA	N05									
FSCONCB	N04									
FSCONCDF	I04									
FSCPYRA	L10									
FSCPYRR	L12									
FSCPYRS	L11									
FSCSSA	L13									
FSCSSR	L15									
FSCSSS	L14									
FSCTIME	L02									
FSDBDTE	D13									

DATA ELEMENT NAME INDEX

Data Element ID = column heading.cell contents (e.g. BQ.B01)

Data Element Name	FS	FA	IC	IA	CC	CA	QC	QA	F1	BQ
FSDIFLAB	R16									
FSDQ	Q24									
FSDUP	R09									
FSEXTANL	I05									
FSF1FLAG	R02									
FSFCDTE	D01									
FSFCTME	D02									
FSFHB	R10									
FSFILE	J03									
FSFSDTE	D03									
FSGENA	Q19									
FSGENB	Q20									
FSGENC	Q21									
FSGENCM	Q23									
FSGEND	Q22									
FSGENDTE	E01	B01								
FSGENTME	E02	B02								
FSHISR	K11									
FSHISS	K10									
FSHLCR	K09									
FSHLCS	K08									
FSHPYRR	K13									
FSHPYRS	K12									
FSHSSR	K15									
FSHSSS	K14									
FSICREF	R03									
FSIDA	Q09									
FSIDB	Q10									
FSIDC	Q11									
FSIDCOM	Q14									
FSIDD	Q12									
FSIDE	Q13									
FSIDEVF	N13									
FSIDEVT	N12									
FSINJVOL	J04									
FSINSTID	J01									
FSINTA	Q05									
FSINTB	Q06									
FSINTC	Q07									
FSINTCM	Q08									
FSIONF	N07									
FSIRAT	N06									
FSISA	M04	C04								
FSISADD	P01									
FSISPH	K05									

DATA ELEMENT NAME INDEX

Data Element ID = column heading.cell contents (e.g. BQ.B01)

Data Element Name	FS	FA	IC	IA	CC	CA	QC	QA	F1	BQ
FSISR	M08	C08								
FSISS	M06	C06								
FSLCA	M01	C01								
FSLCPH	K04									
FSLCR	M03	C03								
FSLCS	M02	C02								
FSMAXS	N09									
FSMBREF	R08									
FSMDREF	R06									
FSMINS	N08									
FSMOIST	I03									
FSMSREF	R05									
FSORIG	H07									
FSPHB	R13									
FSPLDTE	D04									
FSPLS	R14									
FSPMDTE	D05									
FSPMTME	D06									
FSPR	O01									
FSPRCL	O04									
FSPRCU	O05									
FSPRESCR	N14									
FSPRF	O02									
FSPROUT	O06									
FSPSDTE	D07									
FSPYRA	M05	C05								
FSPYRPH	K06									
FSPYRR	M09	C09								
FSPYRS	M07	C07								
FSQFILE	K01									
FSQION	K03									
FSQMTH	K02									
FSQTA	Q15									
FSQTB	Q16									
FSQTC	Q17									
FSQTCOM	Q18									
FSRANG	N10									
FSRANGF	N11									
FSRBREF	R07									
FSRD	P02									
FSRDC	P06									
FSRECALC	R15									
FSRERUN	H05									
FSRF	P04									
FSRR	N01									

DATA ELEMENT NAME INDEX

Data Element ID = column heading.cell contents (e.g. BQ.B01)

Data Element Name	FS	FA	IC	IA	CC	CA	QC	QA	F1	BQ
FSRRC	N02									
FSRRF	N03									
FSRRSTAT	H06									
FSSMPL	H01									
FSSSA	M10	C10								
FSSSADD	O03									
FSSSBF	R11									
FSSSBP	R12									
FSSSPH	K07									
FSSSR	M12	C12								
FSSSS	M11	C11								
FSSTATUS	A02									
FSSULFUR	N15									
FSSURCM	Q04									
FSSURRA	Q01									
FSSURRB	Q02									
FSSURRC	Q03									
FSTRACK	R01									
FSTWTEXT	I01									
FSUPDCNT	E07	B07								
FSUPDDTE	E05	B05								
FSUPDTME	E06	B06								
FSWTEXT	I02									
FTRFFORM	F22									
FTTEMP	G22									
HSID	C01									
ICAADTE			B01							
ICAATME			B02							
ICADDDTE			C03	B03						
ICADDTME			C04	B04						
ICALID			D02							
ICANAL			A02							
ICANALID	B01		A01	A01						
ICANLST			E09							
ICCALA			K01							
ICCALB			K02							
ICCALC			K03							
ICCALD			K04							
ICCANAL			G03							
ICCCCODE			E06							
ICCDATE			G01							
ICCISA			G07							
ICCISR			G09							
ICCISS			G08							
ICCLCA			G04							

DATA ELEMENT NAME INDEX

Data Element ID = column heading.cell contents (e.g. BQ.B01)

Data Element Name	FS	FA	IC	IA	CC	CA	QC	QA	F1	BQ
ICCLCR			G06							
ICCLCS			G05							
ICCOLMMF			E07							
ICCOLMSN			E08							
ICCONC			I07							
ICCPYRA			G10							
ICCPYRR			G12							
ICCPYRS			G11							
ICCSSA			G13							
ICCSSR			G15							
ICCSSS			G14							
ICCTIME			G02							
ICDVCOM			K05							
ICFILE			E10							
ICGENDTE			C01	B01						
ICGENTME			C02	B02						
ICHISR			F11							
ICHISS			F10							
ICHLCR			F09							
ICHLCS			F08							
ICHPYRR			F13							
ICHPYRS			F12							
ICHSSR			F15							
ICHSSS			F14							
ICINJVL			E11							
ICINSTID			E01							
ICINSTMF			E02							
ICINSTMN			E03							
ICISA			H04	C04						
ICISCODE			E04							
ICISPH			F05							
ICISR			H08	C08						
ICISS			H06	C06						
ICLCA			H01	C01						
ICLCPH			F04							
ICLCR			H03	C03						
ICLCS			H02	C02						
ICMRF			I01							
ICPYRA			H05	C05						
ICPYRPH			F06							
ICPYRR			H09	C09						
ICPYRS			H07	C07						
ICQFILE			F01							
ICQION			F03							
ICQMTH			F02							

DATA ELEMENT NAME INDEX

Data Element ID = column heading.cell contents (e.g. BQ.B01)

Data Element Name	FS	FA	IC	IA	CC	CA	QC	QA	F1	BQ
ICRECALC			L01							
ICRF			I06							
ICRSD			I02							
ICRSDC			I03							
ICRSDF			I04							
ICRSDOUT			I05							
ICSMPL			D01							
ICSOLCD			E05							
ICSSA			H10	C10						
ICSSPH			F07							
ICSSR			H12	C12						
ICSSS			H11	C11						
ICSTATUS			A03							
ICUPDCNT			C07	B07						
ICUPDDTE			C05	B05						
ICUPDTME			C06	B06						
IONRATI									F03	
LCICUSE									C01	
LOCDIFF	F11									
MBANALID	B05									
MDANALID	B04									
MEDIA	F06									
MIXRNAME	G06									
MIXTEAM	G07									
MSANALID	B03									
MSFLAG	G13									
NEIGHID	F13									
PC2AADTE					B03					
PC2AATME					B04					
PCBLSEP					J06					
PCCONC			J05							
PCIR					J01					
PCIRF					J04					
PCIRLC					J02					
PCIROUT					J05					
PCIRUC					J03					
PCISADD			J08							
PCOCFORM	G11									
PCPR			J06							
PCPRF			J07							
PCPRLC			J02							
PCPROUT			J04							
PCPRUC			J03							
PCPV					J07					
PCPVC					J09					

DATA ELEMENT NAME INDEX

Data Element ID = column heading.cell contents (e.g. BQ.B01)

Data Element Name	FS	FA	IC	IA	CC	CA	QC	QA	F1	BQ
PCPVF					J08					
PCSNR					J10					
PCSNRC					J12					
PCSNRF					J11					
PCTCON			J01							
PCVOLMCS			J09							
PHBID	C06									
PLFEDEX	G18									
PLJARNBR	G14									
PLPOSHI	G16									
PLPRVBLK	G20									
PLRECBY	G04									
PLSHMETH	G17									
PLSID	C07									
PLSPACE	G15									
PLSRMKS	G19									
PREPCOM	G08									
PREPCOMM	G03									
PREPCOND	G02									
PREPLAB	G01									
PTRFFORM	G12									
QCAADTE							B03			
QCAATME							B04			
QCAD							L03			
QCADCL							L07			
QCADCU							L08			
QCADDDTE							C03	B03		
QCADDTME							C04	B04		
QCAEDTE							B02			
QCAF							L05			
QCALDTE							B01			
QCALID							D02			
QCANALID	B07						A01	A01		
QCANLST							F02			
QCCANAL							H03			
QCCDATE							H01			
QCCISA							H07			
QCCISR							H09			
QCCISS							H08			
QCCLCA							H04			
QCCLCR							H06			
QCCLCS							H05			
QCCONCA							J05			
QCCONCB							J04			
QCCONCDF							E04			

DATA ELEMENT NAME INDEX

Data Element ID = column heading.cell contents (e.g. BQ.B01)

Data Element Name	FS	FA	IC	IA	CC	CA	QC	QA	F1	BQ
QCCONF							M04			
QCCPYRA							H10			
QCCPYRR							H12			
QCCPYRS							H11			
QCCSSA							H13			
QCCSSR							H15			
QCCSSS							H14			
QCCTIME							H02			
QCDBDTE							B05			
QCDQ							O42			
QCF1FLAG							P01			
QCFILE							F03			
QCGENA							O35			
QCGENB							O36			
QCGENC							O37			
QCGENCM							O39			
QCGEND							O38			
QCGENDTE							C01	B01		
QCGENTME							C02	B02		
QCHISR							G11			
QCHISS							G10			
QCHLCR							G09			
QCHLCS							G08			
QCHPYRR							G13			
QCHPYRS							G12			
QCHSSR							G15			
QCHSSS							G14			
QCIDA							O21			
QCIDB							O22			
QCIDC							O23			
QCIDCOM							O26			
QCIDD							O24			
QCIDE							O25			
QCIDEVF							J13			
QCIDEVT							J12			
QCINJVOL							F04			
QCINSTID							F01			
QCINTA							O15			
QCINTB							O16			
QCINTC							O17			
QCINTCM							O18			
QCIONF							J07			
QCIRAT							J06			
QCISA							I04	C04		
QCISADD							L01			

DATA ELEMENT NAME INDEX

Data Element ID = column heading.cell contents (e.g. BQ.B01)

Data Element Name	FS	FA	IC	IA	CC	CA	QC	QA	F1	BQ
QCISPH			-				G05			
QCISR							I08	C08		
QCISS							I06	C06		
QCLCA							I01	C01		
QCLCPH							G04			
QCLCR							I03	C03		
QCLCS							I02	C02		
QCMAXCON							M03			
QCMAXS							J09			
QCMINS							J08			
QCMOIST							E03			
QCORIG							D05			
QCPR							K01			
QCPRCL							K04			
QCPRCU							K05			
QCPRESCR							J14			
QCPRF							K02			
QCPROUT							K06			
QCPYRA							I05	C05		
QCPYRPH							G06			
QCPYRR							I09	C09		
QCPYRS							I07	C07		
QCQFILE							G01			
QCQION							G03			
QCQMTH							G02			
QCQTA							O29			
QCQTB							O30			
QCQTC							O31			
QCQTCOM							O32			
QCRANG							J10			
QCRANGF							J11			
QCRD							L02			
QCRDC							L06			
QCRECALC							P02			
QCRERUN							D03			
QCRF							L04			
QCRR							J01			
QCRRC							J02			
QCRRF							J03			
QCRRSTAT							D04			
QCSADDED							N01			
QCSICON							M01			
QCSMPL							D01			
QCSPDD							N07			
QCSPR							N06			

DATA ELEMENT NAME INDEX

Data Element ID = column heading.cell contents (e.g. BQ.B01)

Data Element Name	FS	FA	IC	IA	CC	CA	QC	QA	F1	BQ
QCSPRCL							N04			
QCSPRCU							N03			
QCSPRL							N05			
QCSRECV							N02			
QCSSA							I10	C10		
QCSSADD							K03			
QCSSPH							G07			
QCSSR							I12	C12		
QCSSS							I11	C11		
QCSTATUS							A02			
QCSULFUR							J15			
QCSURCM							O12			
QCSURRA							O09			
QCSURRB							O10			
QCSURRC							O11			
QCTICON							M02			
QCTWTEXT							E01			
QCTYPE							D06			
QCUPDCNT							C07	B07		
QCUPDDTE							C05	B05		
QCUPDTME							C06	B06		
QCWTEXT							E02			
RBANALID	B06									
RRT									F04	
SAMPTYPE	F03									
SCANRNG									F02	
SITENBR	F04									
SOILCOMP	F16									
SPFORM	G05									
SPLIT	G10									
SSBIDF	C04									
SSBIDP	C05									
STREET	F05									
S_FLAG									D01	
S_FLAG5									D05	
TEAMNBR	F14									
TRAKCOM	G09									
TRTEMP	G23									
TUBENBR	F17									
XACTUAL	F09									
XCOORD	F07									
YACTUAL	F10									
YCOORD	F08									

APPENDIX B

Names of Equivalent Data Elements Contained in Multiple Files

LOVE CANAL HABITABILITY STUDY
NAMES OF "LIKE" DATA ELEMENTS CONTAINED IN MULTIPLE FILES

FIELD DESCRIPTION	FS	QC	F1	IC	CC
Keys					
Analysis Lab Sample Id	ALANALID	QCANALID	F1ANALID	ICANALID	CCANALID
Project Field Sample Id (HS #)	HSID	QCSMPL	F1SMPL	ICSAMPL	CCSMPL
Chronology					
Analysis Lab Login Date	FSALDTES	QCALDTE			
Analysis Lab Analysis Date	FSAADTE	QCAADTE	F1AADTE	ICAADTE	CCAADTE
Analysis Lab Analysis Time	FSAATME	QCAATME	F1AATME	ICAATME	CCAATME
Data Xfer Tracking					
Labdata Gen Date	FSGENDTE	QCGENDTE	F1GENDTE	ICGENDTE	CCGENDTE
Labdata Gen Time	FSGENTME	QCGENTME	F1GENTME	ICGENTME	CCGENTME
DB Add Date	FSADDDTE	QCADDDTE		ICADDDTE	CCADDDTE
DB Add Time	FSADDTME	QCADDTME		ICADDTME	CCADDTME
DB Most Recent Update Date	FSUPDDTE	QCUPDDTE		ICUPDDTE	CCUPDDTE
DB Most Recent Update Time	FSUPDTME	QCUPDTME		ICUPDTME	CCUPDTME
DB Update Count	FSUPDCNT	QCUPDCNT		ICUPDCNT	CCUPDCNT
Analysis Lab Sample Login Data					
Project Sample Id	FSSMPL	QCSMPL		ICSMPL	CCSMPL
Analytic Laboratory Id	FSALID	QCALID		ICALID	CCALID
Analysis Lab Sample Extraction Data					
Target Weight to Extract	FSTWTEXT	QCTWTEXT			
Weight Extracted (gm)	FSWTEXT	QCWTEXT	F1WTEXT		
Percent Moisture	FSMOIST	QCMOIST	F1MOIST		
Concentration Dilution Factor	FSCONCDF	QCCONCDF	F1CONCDF		

LOVE CANAL HABITABILITY STUDY
NAMES OF "LIKE" DATA ELEMENTS CONTAINED IN MULTIPLE FILES

FIELD DESCRIPTION	FS	QC	F1	IC	CC
Analysis Lab Injection Data					
GC/MS Instrument Id	FSINSTID	QCINSTID		ICINSTID	CCINSTID
GC/MS Analyst	FSANLST	QCANLST	F1ANLST	ICANLST	CCANLST
GC/MS Datafile Id	FSFILE	QCFILE	F1DFILE	ICFILE	CCFILE
Injection Volume	FSINJVOL	QCINJVOL		ICINJVL	CCINJVL
Analysis Lab Interpretation Data					
GC/MS Shift Results File Name	FSQFILE	QCQFILE		ICQFILE	CCQFILE
Quantitation Method Flag	FSQMTH	QCQMTH		ICQMTH	CCQMTH
LCIC Quantition Ion Selection	FSQION	QCQION		ICQION	CCQION
Peak Height Data					
Peak Height, by 8 LCICs, By 3 Ions	FSLCPH	QCLCPH		ICLCPH	CCLCPH
Peak Height, by 5 Int. Stds. (Primary Ion)	FSISPH	QCISPH		ICISPH	CCISPH
Peak Height, Pyrene-D10 (Secondary Ion)	FSPYRS	QCPYRS		ICPYRS	CCPYRS
Peak Height, by 3 Surrogates (Primary Ion)	FSSSPH	QCSSPH		ICSSPH	CCSSPH
Scan for Peak Height by 8 LCICs, by 3 Ions	FSHLCS	QCHLCS		ICHLCS	CCHLCS
Retention Time for Peak Height by 8 LCICs, by 3 Ions	FSHLCR	QCHLCR		ICHLCR	CCHLCR
Scan for Peak Height, by 5 Internal Standards	FSHISS	QCHIS		ICHISS	CCHISS
Retention Time for Peak Height, by 5 Internal Standards	FSHISR	QCHISR		ICHISR	CCHISR
Scan for Peak Height for Pyrene-D10	FSHPYRS	QCHPYRS		ICHPYRS	CCHPYRS
Retention Time for Peak Height, for Pyrene-D10	FSHPYRR	QCHPYRR		ICHPYRR	CCHPYRR

LOVE CANAL HABITABILITY STUDY
NAMES OF "LIKE" DATA ELEMENTS CONTAINED IN MULTIPLE FILES

FIELD DESCRIPTION	FS	QC	F1	IC	CC
Scan for Peak Height, by 3 Surrogates	FSHSSS	QCHSSS		ICHSSS	CCHSSS
Retention Time for Peak Height, by 3 Surrogates	FSHSSR	QCHSSR		ICHSSR	CCHSSR
Correction Flags					
Analysis Lab Analysis Date	FSCDATE	QCCDATE		ICCDATE	CCCDATE
Analysis Lab Analysis Time	FSCTIME	QCCTIME		ICCTIME	CCCTIME
Analyst	FSCANAL	QCCANAL		ICCANAL	CCCANAL
Area, by 8 LCICs, by 3 Ions	FSCLCA	QCCLCA		ICCLCA	CCCLCA
Scan, by 8 LCICs, by 3 Ions	FSCLCS	QCCLCS		ICCLCS	CCCLCS
Retention Time, by 8 LCICs, by 3 Ions	FSCLCR	QCCLCR		ICCLCR	CCCLCR
Area, by 5 Int. Stds., (Primary Ion)	FSCISA	QCCISA		ICCISA	CCCISA
Scan, by 5 Int. Stds., (Primary Ion)	FSCISS	QCCISS		ICCISS	CCCISS
Retention Time, by 5 Int. Stds., (Primary Ion)	FSCISR	QCCISR		ICCISR	CCCISR
Area, Pyrene-D10 (Secondary Ion)	FSCPYRA	QCCPYRA		ICCPYRA	CCCPYRA
Scan, Pyrene-D10 (Secondary Ion)	FSCPYRS	QCCPYRS		ICCPYRS	CCCPYRS
Retention Time, Pyrene-D10 (Secondary Ion)	FSCPYRR	QCCPYRR		ICCPYRR	CCCPYRR
Area, By 3 Surrogates (Primary Ion)	FSCSSA	QCCSSA		ICCSSA	CCCSSA
Scan, By 3 Surrogates (Primary Ion)	FSCSSS	QCCSSS		ICCSSS	CCCSSS
Retention Time, By 3 Surrogates (Primary Ion)	FSCSSR	QCCSSR		ICCSSR	CCCSSR

LOVE CANAL HABITABILITY STUDY
NAMES OF "LIKE" DATA ELEMENTS CONTAINED IN MULTIPLE FILES

FIELD DESCRIPTION	FS	QC	F1	IC	CC
Analysis Raw Data (After Corrections, if any)					
Area, by 8 LCICs, by 3 Ions	FSLCA	QCLCA		ICLCA	CCLCA
Scan, by 8 LCICs, by 3 Ions	FSLCS	QCLCS		ICLCS	CCLCS
Retention Time, by 8 LCICs, by 3 Ions	FSLCR	QCLCR		ICLCR	CCLCR
Area, by 5 Int. Stds. (Primary Ion)	FSISA	QCISA		ICISA	CCISA
Area, Pyrene-D10 (Secondary Ion)	FSPYRA	QCPYRA		ICPYRA	CCPYRA
Scan, by 5 Int. Stds. (Primary Ion)	FSISS	QCISS		ICISS	CCISS
Scan, Pyrene-D10 (Secondary Ion)	FSPYRS	QCPYRS		ICPYRS	CCPYRS
Retention time, by 5 Int. Stds. (Primary Ion)	FSISR	QCISR		ICISR	CCISR
Retention time, Pyrene-D10 (Secondary Ion)	FSPYRR	QCPYRR		ICPYRR	CCPYRR
Area, by 3 Surrogates (Primary Ion)	FSSSA	QCSSA		ICSSA	CCSSA
Scan, by 3 Surrogates (Primary Ion)	FSSSS	QCSSS		ICSSS	CCSSS
Retention Time, by 3 Surrogates (Primary Ion)	FSSSR	QCSSR		ICSSR	CCSSR
LABDATA Computations for Field and QC Samples					
Relative Retention Time, by 8 LCICs (Quantitation Ion)	FSRR	QCRR			
Relative Retention Time Criteria, by 8 LCICs	FSRRC	QCRRC			
Flag for Rel. Ret. Time Out of Criteria, by 8 LCICs	FSRRF	QCRRF	RRT		
Pre-criteria Concentration, by 8 LCICs	FSCONCB	QCCONCB			
Criteria Concentration, by 8 LCICs	FSCONCA	QCCONCA	CONC		
Ion Ratio, by 8 LCICs	FSIRAT	QCIRAT			

LOVE CANAL HABITABILITY STUDY
NAMES OF "LIKE" DATA ELEMENTS CONTAINED IN MULTIPLE FILES

FIELD DESCRIPTION	FS	QC	F1	IC	CC
Flag for All Ions Being Present, by 8 LCICs	FSIONF	QCIONF	ALLIONS		
Minimum Scan Number of 3 Ions, by 8 LCICs	FSMINS	QCMINS			
Maximum Scan Number of 3 Ions, by 8 LCICs	FSMAXS	QCMAXS			
Scan Range (Max-Min), by 8 LCICs	FSRANG	QCRANG			
Flag for Scan range >2, by 8 LCICs	FSRANGF	QCRANGF	SCANRNG		
Ion Ratio % Dev. from Theoretical Values, by 8 LCICs	FSIDEVT	QCIDEVT			
Flag for Ion ratio % Dev. Out of Criteria, by 8 LCICs	FSIDEVF	QCIDEVF	IONRATI		
Flag for Analysis Pre-screen	FSPRESCR	QCPRESCR			
Flag for Sulphur Cleanup Performed	FSSULFUR	QCSULFUR			
LABDATA Computations for Surrogate Standards					
% Recovery by 3 Surrogates	FSPR	QCPR			
Flag for % Rec. Out of Criteria	FSPRF	QCPRF			
Amount of Surrogate added(ng)	FSSSADD	QCSSADD			
% Recovery Criteria lower limit	FSPRCL	QCPRCL			
% Recovery Criteria upper limit	FSPRCU	QCPRCU			
Number of % Rec. Out of Criteria	FSPROUT	QCPROUT			
LABDATA Computations for Internal Standards					
Internal Standard Quantity Added (in nanograms)	FSISADD	QCISADD			
Ret. Time Difference From CC Val	FSRD	QCRD			
Area Difference % From CC Val	FSAD	QCAD			
Flag for Ret. Time Out of Criteria	FSRF	QCRF			

LOVE CANAL HABITABILITY STUDY
NAMES OF "LIKE" DATA ELEMENTS CONTAINED IN MULTIPLE FILES

FIELD DESCRIPTION	FS	QC	F1	IC	CC
Flag for Area Out of Criteria	FSAF	QCAF			
Retention Time Difference Criteria	FSRDC	QCRDC			
Area % Diff. Crit. lower limit	FSADCL	QCADCL			
Area % Diff. Crit. upper limit	FSADCU	QCADCU			

APPENDIX C

Formulas for Computed Data Elements

FORMULAS

This appendix contains the formulas used by LabData and the Integrated Data Base for chemistry computations. This presentation is oriented toward the computations from a data processing perspective. The equations are presented in the form used for the data base calculations. The equations may not appear to be equivalent to those in the SOW but are in fact the same. For a fuller treatment from a chemistry perspective, refer to the Love Canal Habitability Study--Soil Sample Laboratory Analysis Quality Assurance Project Plan.

Terminology

The objective of the chemistry method was to measure concentrations of the eight Love Canal Indicator Chemicals (LCICs). These eight compounds are always numbered as follows:

1 = 1,2-Dichlorobenzene	DCB
2 = 1,2,4-Trichlorobenzene	TCB
3 = 1,2,3,4-Tetrachlorobenzene	TeCB
4 = 2-Chloronaphthalene	CNP
5 = Alpha-BHC	A-BHC
6 = Delta-BHC	D-BHC
7 = Beta-BHC	B-BHC
8 = Gamma-BHC	G-BHC

All concentrations are in parts per billion (ppb).

In addition to the LCICs, concentrations (and percent recovery) for three surrogate standard (S.S.) compounds are computed. The three surrogates are always numbered as follows:

1 = 1,4-Dibromobenzene	DBB
2 = 2,4,6-Tribromobiphenyl	TBBP
3 = 1,2,4,5-Tetrabromobenzene	QBB

Associated with each LCIC and surrogate is an internal standard. For each injection into the GC/MS/SIM, the internal standards have a known concentration so that variations in injection volume and instrument response are compensated. There are five internal standards, and they are always numbered as follows:

1 = D4-1,4-Dichlorobenzene	IS1
2 = D8-Naphthalene	IS2
3 = D10-Acenaphthene	IS3
4 = D10-Phenanthrene	IS4
5 = D10-Pyrene	IS5

The associations of the LCICs and surrogates to the internal standards (I.S.) are given below:

Compound	Associated I.S. Number
LCIC #1	1
LCIC #2	2
LCIC #3	3
LCIC #4	3
LCIC #5	4
LCIC #6	4
LCIC #7	4
LCIC #8	4
S.S. #1	2
S.S. #2	4
S.S. #3	5

The basic units of direct measurement in the GC/MS/SIM itself are area, peak height, retention time, and scan number. Area and peak height are strictly relative units within the instrument. Retention time is measured in seconds, and scan numbers are half-second intervals of retention time. The predominant, and preferred, method for computing concentrations uses the area measurement. Peak height is used in instances of excessive interference.

For each LCIC, three ions are measured so that there are potentially three areas, retention times, and scan numbers for each of the eight LCICs. These three ions are classified as primary, secondary, and tertiary. One ion is measured for each I.S. and S.S., except a secondary ion is also measured for D10-Pyrene. The three ions are classified as primary, secondary, and tertiary in relation to their relative abundance. With some exceptions, the LCIC concentrations are computed using the primary ion.

There are some basic relationships among GC/MS/SIM analyses that are critical to the computations. The GC/MS/SIM instrument is first calibrated using a five-point initial calibration (I.C.). Each 12-hour analytical run ("shift") begins with a continuing calibration/performance check (CC/PC1) that directly relates to the I.C. Each analysis in the 12-hour shift relates directly to the CC/PC1. At the end of a 12-hour shift there is a second performance check (PC2) that relates directly to the CC/PC1. The QAPP allows either one calibration per 12-hour shift or two calibrations per 16-hour shift.

Calibration Computations

There are two types of calibrations used: an initial calibration (I.C.) performed at five different concentrations and a

continuing calibration/performance check performed at the second lowest I.C. concentration. The five I.C. concentrations are:

0.05
0.10
0.50
1.0
2.0

The primary numbers computed during the calibrations are relative response factors (RRFs). RRFs are computed for each LCIC and surrogate. They establish the relative responses of the LCICs and surrogates to the internal standards.

The RRFs are computed as follows:

$$RRF = AREA / ISAREA / ICCONC, \quad (1)$$

where:

RRF = relative response factor,
AREA = LCIC or S.S. primary ion area,
ISAREA = the associated I.S. area, and
ICCONC = the appropriate calibration concentration = (ICCONC is the concentration of LCIC or S.S. divided by concentration of I.S.)

RRFs are computed for the primary ions of LCICs and S.S.'s for each of the five initial calibration runs. Over the five I.C. runs, a mean RRF and percent relative standard deviation is computed for each LCIC and S.S. The mean RRF is computed as:

$$RRFBAR = \left(\sum_{i=1}^{5} RRF_i\right) / 5, \quad (2)$$

where:

RRFBAR = mean relative response factor for an LCIC or S.S.,
i = I.C. number 1 to 5, and
RRFi = the RRF for the LCIC or S.S. for the i^{th} I.C. point

$$SD = \left[\sum_{i=1}^{n} (RRF_i - RRFBAR)^2 \right]^{1/2} / (n-1) \qquad (3)$$

where:

RRFBAR = mean relative response factor for an LCIC or S.S.,
i = I.C. number 1 to 5, and
RRFi = the RRF for the LCIC or S.S. for the i^{th} I.C. point

The %RSD is computed as:

$$\%RSD = SD / RRFBAR * 100, \qquad (4)$$

where:

%RSD = the percent relative standard deviation for the LCIC or S.S.,
RRFBAR = mean RRF, and
SD = standard deviation of the 5 RRFs for the LCIC or S.S.

Stringent QA/QC criteria are set for the %RSD values because it measures the linearity of the instrument response. The RRFBAR values are compared to the RRFs computed in the CC/PC1 as follows:

$$\%D = \left| (CCRRF - RRFBAR) / RRFBAR \right| * 100, \qquad (5)$$

where:

%D = CC/PC1 percent deviation for an LCIC or S.S.,
CCRRF = CC/PC1 RRF for the LCIC or S.S., and
RRFBAR = mean RRF from the I.C.

QA/QC criteria are set for the %D to determine if the GC/MS/SIM is still in calibration. The CCRRF is computed using equation (1) and an ICCONC value of 0.10.

The continuing calibration relative retention times (CCRR) are computed for each ion of each LCIC. For Finnigan GC/MS instruments,

$$CCRR = SCAN / ISSCAN, \quad (6)$$

where:

CCRR = relative retention time for a given LCIC and ion,
SCAN = the scan value of the given LCIC and ion, and
ISSCAN = the scan value of the appropriate I.S.

For Hewlett Packard GC/MS instruments,

$$CCRR = RT / ISRT, \quad (7)$$

where:

RT = retention time (seconds) of the given LCIC and ion, and
ISRT = retention time (seconds) of the appropriate I.S.

The CCRR formulas are different for the two manufacturers because of differences in quantitation report formats.

The CCRR values are used in the relative retention time LCIC identification criteria that is discussed later. Also, the I.S. areas and scan value for the CC/PC1 are used in I.S. QA/QC criteria for the subsequent analyses.

Performance Check Computations

The CC/PC1 and PC2 analyses are used to check instrument sensitivity. The measures of instrument sensitivity are ion ratios, specific chromatographic signal-to-noise ratios, and chromatographic signal separation measures.

The performance check ion ratios (PCIR) are computed for CC/PC1 and PC2 for each LCIC and for D10-Pyrene (I.S. #5). Except for LCIC #3 (1,2,3,4-Tetrachlorobenzene), the PCIR is computed as secondary ion area divided by primary ion area. For LCIC #3, PCIR is computed as primary ion divided by secondary ion.

The chromatographic values cannot be computed from other data.

Concentration Computations

LCIC dry weight concentrations are computed as:

$$CONC = AREA / ISAREA / CCRRF / WTEXT / MSTRFACT * ISADDED * CDFACTOR, \quad (8)$$

where:

CONC = LCIC concentration in ng/gm,
AREA = LCIC quantitation primary ion area,
ISAREA = associated I.S. area,
CCRRF = continuing calibration relative response factor for the quantitation primary ion,
WTEXT = weight extracted in grams,
MSTRFACT = adjustment for percent moisture,
ISADDED = internal standard amount added, in nanograms, and
CDFACTOR = concentration/dilution factor (usually 1.0).

MSTRFACT is computed as:

$$MSTRFACT = (100 - PCTMSTR) / 100, \quad (9)$$

where:

PCTMSTR = sample percent moisture.

In almost all cases, the primary ion is used for quantitation.

The Form I concentrations are either values computed using equation (6) or "ND" (non-detect) if one or more of the LCIC identification criteria are not met. The four identification criteria are:

1. All three ions are present.
2. The primary, secondary, and tertiary ions of each LCIC must maximize within $\pm$ two scans of each other. (The range of scan numbers for the three ions is less than or equal to 2.)
3. The secondary to primary ion ratios are within 20% of the theoretical value.
4. The quantitation ion is within 0.005 relative retention time (RRT) units of the same ion in the CC/PC1 run.

Method/Holding Blanks

The Method/Holding blanks have Form I concentrations computed and also have concentrations computed for all three ions without any identification criteria applied. These concentrations for all

three ions are reported on Form IV and indicate interference in any ion of any LCIC.

Matrix Spike/Matrix Spike Duplicates

The complete matrix spike/matrix spike duplicate (MS/MSD) analysis consists of three extractions from the same sample:

- the sample with no LCICs added (the "native sample"),
- the sample with approximately 5 ng/gm of LCICs added (the "matrix spike"), and
- a second extraction of the sample with approximately 5 ng/gm (the "matrix spike duplicate") of LCICs added.

Form I concentrations are reported for all three extractions. In addition, computations involving all three extractions are performed. These are matrix spike percent recovery (MSPR) and matrix spike relative percent deviation (MSRPD). A major difference between the Form I and the Form III concentrations is that Form I concentrations are reported as dry weights and Form III concentrations are reported as wet weights. Wet weight concentrations are computed using equation (8) with the MSTRFACT term removed. The identification criteria are different from those used to report results on Form I. The MS and MSD calculations reported on Form III are made using only the relative retention time for the native sample. The MS and MSD percent recoveries are computed by:

$$MSPR = (MSCONC - FSCONC) / MSAMTADD * 100, \quad (10)$$

where:

MSPR = MS or MSD percent recovery,
MSCONC = MS or MSD wet weight concentration (result),
FSCONC = native sample wet weight concentration (result) with only the RRT identification criteria applied, and
MSAMTADD = concentration of LCICs added to the MS or MSD at extraction.

The MSAMTADD is nominally 5 ng/gm, but it needs to be adjusted for the actual weight extracted. This adjustment is done by:

$$MSAMTADD = MSAMT * CRITWEXT / MSWTEXT, \quad (11)$$

where:

MSAMTADD = concentration of LCICs added to the MS or MSD, in ng/gm,
MSAMT = nominal concentration added (5 ng/gm in this study),
CRITWEXT = method criteria weight to extract (20 gm), and
MSWTEXT = actual weight extracted in the MS or MSD.

The MS/MSD relative percent deviation (MSRPD) is computed by:

$$MSRPD = (MSPR - MSDPR) / (MSPR + MSDPR) * 200, \quad (12)$$

where:

MSRPD = the MS/MSD relative percent deviation,
MSPR = matrix spike percent recovery, and
MSDPR = matrix spike duplicate percent recovery.

Surrogate Percent Recovery

The surrogate percent recovery is computed by:

$$SSPR = AREA / ISAREA / CCRRF / SSADDED * ISADDED * CDFACTOR * 100 \quad (13)$$

where:

SSPR = surrogate percent recovery,
AREA = surrogate primary ion area,
ISAREA = internal standard primary ion area,
CCRRF = relative response factor from the CC/PC1,
SSADDED = amount of surrogate added, in ng,
ISADDED = amount of internal standard added, in ng, and
CDFACTOR = concentration/dilution factor (usually 1.0).

Peak Heights

The LCIC chemistry methodology permits the chemists to use peak heights of the GC/MS response curves instead of area if there is chemical or matrix interference that makes the areas unreliable measures. All of the computation formulas can be used by substituting peak height values for areas. This is possible because the areas and peak heights are unitless, relative measures.

Peak height concentration computations require relative response factors computed using peak heights in the CC/PC1. For any sample, the concentrations require peak heights for the particular LCIC quantitation ion and the applicable internal standard.

APPENDIX D

Box Plot - A Graphic Representation of Analytical Results

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Box Plot - A Graphic Representation of Analytical Results

Box plots were used to visually compare data across laboratories or other stratifiers of interest. Although these graphic representations are not a substitute for formal statistical analysis, they should be generally consistent with the statistical analysis and accordingly provide a qualitative cross-check of the results of the statistical comparisons.

An example of a box plot is shown in Figure D-1. This box plot shows one page (one surrogate) of surrogate recoveries. The vertical axis is the percent recovery. The horizontal axis is the analytical laboratory. The box includes the middle 50 percent of the data. The line in the box marks the median, or 50th percentile; 25 percent of the data are included in the part of the box above the median line, and 25 percent are in the part below the median line.

The upper "whisker" (vertical line above the box) extends to the largest non-extreme value (the interpretation of "extreme" is based on a relationship with the normal [Gaussian] distribution). The extreme values are plotted with asterisks and the more extreme with circles. Those extreme values that lie off the scale are printed at the top of the figure.

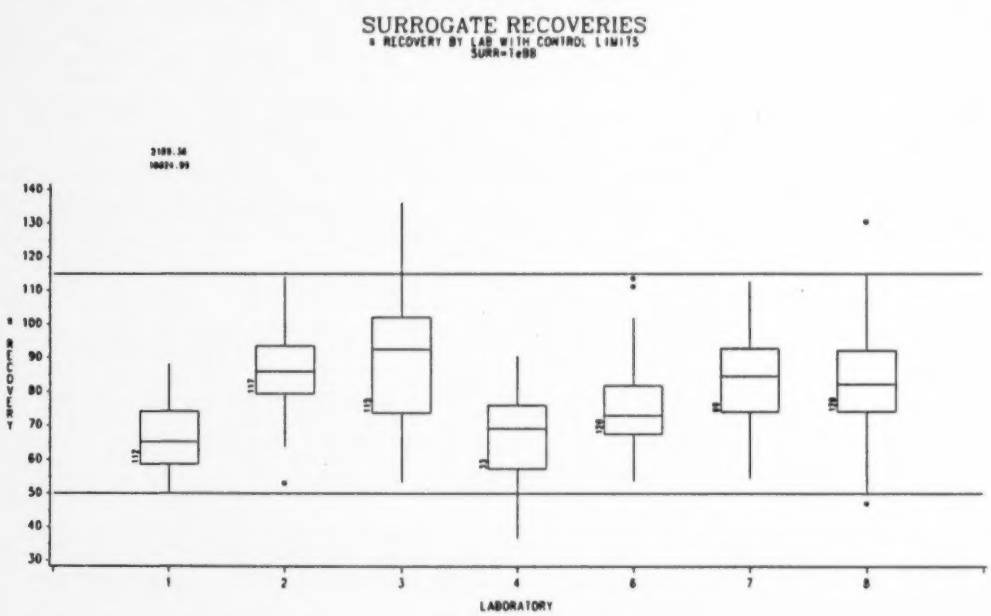

Figure D-1
Example of a Box Plot